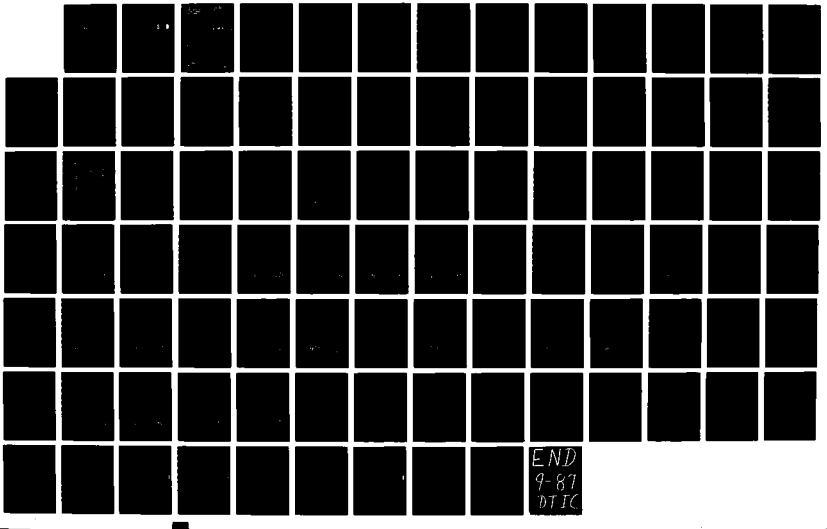
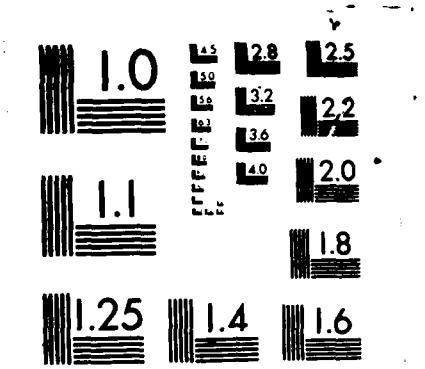
AD-A183 579 ESTIMATION OF MELTING POINT(U) ARIZONA UNIV TUCSON S H YALKOWSKY ET AL. 23 FEB 87 DAMD17-85-C-5005 1/1

UNCLASSIFIED F/G 7/3 NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

DTIC FILE COPY

AD-A183 579

AD_____

ESTIMATION OF MELTING POINT

ANNUAL AND FINAL REPORT

DTIC
ELECTE
AUG 05 1987
S D
D

Samuel H. Yalkowsky
Robert Abramowitz
Peter D. Tsakanikas

February 23, 1987

Supported by

U.S. ARMY MEDICAL RESEARCH AND DEVELOPMENT COMMAND
Fort Detrick, Frederick, Maryland 21701-5012

Contract No. DAMD17-85-C-5005

University of Arizona
Tucson, Arizona 85721

"Contracting Officer's Representative:
David H. Rosenblatt, Ph.D.
U.S. Army Biomedical Research
and Development Laboratory
Fort Detrick, Frederick, MD 21701-5010"

DOD DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorized documents.

87 8 4 076

SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION: Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT: Approved for public release; Distribution unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S)
6a. NAME OF PERFORMING ORGANIZATION: University of Arizona; 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION
6c. ADDRESS (City, State, and ZIP Code): Tucson, Arizona 85721	7b. ADDRESS (City, State, and ZIP Code)
8a. NAME OF FUNDING/SPONSORING ORGANIZATION: U.S. Army Medical Research and; 8b. OFFICE SYMBOL (If applicable): Development Command	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: DAMD17-85-C-5005
8c. ADDRESS (City, State, and ZIP Code): Fort Detrick, Frederick, Maryland 21701-5012	10. SOURCE OF FUNDING NUMBERS: PROGRAM ELEMENT NO. 62720A; PROJECT NO. 3EL-62720A835; TASK NO. AA; WORK UNIT ACCESSION NO. 024

11. TITLE (Include Security Classification)
Estimation of Melting Point

12. PERSONAL AUTHOR(S)
Yalkowsky, Samuel H., Abramowitz, Robert, Tsakanikas, Peter D.

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Annual and Final	FROM 84/11/15 TO 86/11/30	1987 Feb. 23	88

16. SUPPLEMENTARY NOTATION

17 COSATI CODES			18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	
07	04		Melting Point
07	02		

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Two equations have been developed for the estimation of the melting points, TM, of rigid aromatic and flexible aliphatic organic compounds. These compounds include alkyl, halo, cyano, nitro, hydroxo substituted benzenes, aromatic polycyclics and branched and unbranched paraffins. The estimation was accomplished through use of thermodynamic parameters related to melting. The approach includes both additive and non-additive constitutive properties of the molecules.

(Keywords)

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT: ☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT ☐ DTIC USERS	21. ABSTRACT SECURITY CLASSIFICATION: Unclassified
22a. NAME OF RESPONSIBLE INDIVIDUAL: Ms. Virginia Miller	22b. TELEPHONE (Include Area Code): (301) 662-6216; 22c. OFFICE SYMBOL: SGRD-RMI-S

DD FORM 1473, 84 MAR — 83 APR edition may be used until exhausted. All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE

TABLE OF CONTENTS

Accesion For
NTIS CRA&I
DTIC TAB
Unannounced
Justification
By
Distribution /
Availability Codes
Dist Avail and/or Special
A-1

DTIC COPY INSPECTED 6

SECTION I-PURPOSE

The purpose of this study is 1) to determine which additive and non-additive molecular properties contribute most significantly to melting point and 2) to develop techniques by which the melting point of rigid non-hydrogen bonding, rigid hydrogen bonding and flexible organic compounds can be estimated on the basis of their chemical structures.

Although melting point is by far the most commonly reported property of organic compounds, it is among the least understood from a structure-property point of view. In spite of the tremendous amount of available data, there are few guidelines for understanding the relationship between melting point and chemical structure.

The melting point of a compound is a major determinant of many of its other physical chemical properties. Melting point has been quantitatively related to the solubility of organic compounds (1,2). From the environmental point of view for instance, the latter is a key property one needs to know in chemical clean-up processes. For the solubility to be estimated properly, it is necessary to know the melting point and either the heat or entropy of fusion of the compound. Since it is sometimes important to know these parameters for compounds that do not exist or that are not available in sufficient purity to use for analytical measurements, it would be useful to be able to estimate them from the chemical structure.

SECTION II-METHODS

LITERATURE VALUES OF ORGANIC COMPOUNDS

The literature values for the melting points of approximately 1380 rigid aromatic compounds and 400 flexible aliphatic compounds have been obtained (3,4,5). These include both hydrogen bonding and non-hydrogen bonding compounds.

DATABASE SYSTEM

A database for all of the organic chemicals used in this study has been developed. The database contains the melting point, enthalpy of fusion, entropy of fusion of each compound and other structural information. The database system is a computer-based record-keeping system to record and maintain information. The database system allows easy manipulation of melting point data. The database has been developed on dBASE II software and updated to dBASE III using DEC Rainbow computers.

The database includes the maximum molecular lengths of all compounds in the study. The maximum molecular lengths were

obtained from molecular models (Fisher Scientific) using standard geometry. These molecular lengths along with the van der Waals volume (VOLUME) of a molecule are needed in order to calculate the eccentricity of the molecule. The database also includes the polarizability (ALPHA) and the scalar sum of the group dipole moments (SUMDM). The group dipole moments are found in Table 1. The polarizability was calculated from the group values of Ferguson (6) as found in Table 2. The van der Waals volumes are from Edward (7) and are contained in Table 3. A program was written in dBASE III to calculate and store these variables in the database. This program is contained in Appendix A. Appendix B contains the name of each rigid compound in the database along with the melting point, molecular length, molecular weight, VOLUME, ALPHA, SUMDM and symmetry number (SIGMA). The data in Appendix B are sorted by molecular weight in order to obtain easy access for any compound. Appendix C contains the melting properties of all flexible molecules used in this study thus far, along with their flexibility and symmetry numbers.

EXPERIMENTAL DATA

Approximately 75 compounds of high purity have been obtained. Forty-eight of these compounds have been analyzed on a Dupont differential scanning calorimeter (DSC), and from the DSC analysis we have obtained the melting point, the enthalpy of fusion and the purity of the compounds. The output of the DSC analyses for representative compounds are shown in Appendix D.

SECTION III-RESULTS AND DISCUSSION

NON-HYDROGEN BONDING COMPOUNDS

An equation has been developed for estimating the melting points of rigid non-hydrogen bonding aromatic compounds. These compounds include the alkyl, halo, nitro and cyano benzenes and a number of polycyclic aromatic hydrocarbons.

ALPHAL is the logarithm of the polarizability of the molecule (note: in this report "log" always refers to the base 10). The polarizability of a molecule is a measure of the size of its electron cloud. It has units of volume and is roughly proportional to the volume of the molecule. The larger the electron cloud, the more easily it is distorted. The polarizability of a molecule can be related to the van der Waals dispersion and induction forces. Non-hydrogen bonding molecules are held together primarily by these van der Waals (dipolar, induction and dispersion) forces.

The net dipole moment of a molecule is a measure of its ability to interact electrostatically with neighboring dipoles and its ability to induce a dipole in a neighboring molecule by polarization of the electron cloud of the

neighboring molecule. This quantity is thus important in both induction and dipolar interactions. At close distances of separation, however, it is not reasonable to expect the net molecular dipole moment to be the primary determinant of dipolar interactions. At close distances, the various portions of neighboring molecules can interact electrostatically as though they were independent dipoles. Thus, it is appropriate to consider SUMDM, which is the scalar sum of all group dipole moments of a molecule, rather than the net dipole moment of a molecule. The group contributions to the dipole moment of a molecule were obtained from Smyth and are listed in Table 1.

SIGMAL is the logarithm of the rotational symmetry number of the molecule. The rotational symmetry number is defined as the number of orientations of the molecule indistinguishable from a reference position. A methyl group is treated as symmetrical in this framework. In calculating the symmetry number of a molecule, the following groups are considered to be equal in size: methyl, chloro, bromo and cyano. The iodo, nitro and fluoro groups are not considered to be equal because of their size differences from the other groups. From an intuitive point of view, molecular symmetry is a measure of the probability that a freely rotating molecule will be oriented in a manner suitable for incorporation into a crystal. This definition of SIGMAL could help explain the positional disordering of crystals.

The eccentricity of a molecule is defined as the ratio of the maximum molecular length to the mean molecular diameter.

$$\text{Eccentricity} = \frac{\text{maximum molecular length}}{\text{mean molecular diameter}} \qquad (1)$$

The mean molecular diameter is calculated as the diameter of a sphere occupied by the total volume of the molecule. Equation 2 gives the formula for the volume of a sphere.

$$\text{VOLUME} = \frac{4\pi r^3}{3} \qquad (2)$$

Rearrangement of equation 2 and substitution of DIAMETER/2 for the radius gives equation 3.

$$\text{DIAMETER} = 2\left(\frac{3(\text{VOLUME})}{4\pi}\right)^{1/3} \qquad (3)$$

The total volume of the molecule is calculated from the group contribution values from Edward (7). The maximum molecular length of a molecule has been determined from molecular models.

EXPAN, which is the eccentricity of the molecule to the third power, can be related to the differences in packing efficiency between the liquid and the crystal. EXPAN can now be calculated by substituting equation 3 into equation 1 and taking the entire quantity to the third power.

$$EXPAN = \frac{\pi(LENGTH)^3}{6(VOLUME)} \qquad (4)$$

The greater the EXPAN value associated with a molecule, the greater the increase in volume required for the rotational freedom that occurs on melting. EXPAN is therefore particularly important for polycyclic molecules.

The variables PACK1, PACK8 and PACK9 are indicator variables to indicate various structural features of the molecule. Thirteen different structural features such as meta, ortho and para substituted benzenes were tested. From statistical analysis three of these indicator variables were significant. PACK1 refers to any hexa-substituted benzene molecule, such as hexabromobenzene or 1,2,3-trichloro-4,5,6-triiodobenzene. PACK8 is any para-disubstituted benzene molecule while PACK9 refers to a 1,2,4,5-tetrasubstituted benzene compound. These indicator variables can be thought of as factors that influence the enthalpy of melting by increasing the packing efficiency of the crystal through decreasing the separation distance between interacting groups of complex molecules.

The variables CBR and CBRBIPH are indicator variables that help to describe polyaromatic molecules. CBR refers to the number of bridgehead carbons in the molecule. A bridgehead carbon is any carbon that is shared by more than one aromatic ring. CBRBIPH refers to the number of carbons in a molecule involved in a biphenyl linkage. For example biphenyl has two such carbon atoms.

Statistical analysis on part of the data was performed using the statistical programs in SAS (Statistical Analysis System). The variables used in the multiple regression models are described in Table 4.

The first regression analysis includes only halo and alkyl benzenes without fluorine atoms. The equation developed to predict the melting point of these compounds includes both additive and non-additive constitutive properties of the molecule. A summary of the regression analysis is contained

in Table 5. All of the parameters in the equation are statistically significant. This can be seen from an evaluation of the T test that is shown in Table 5. The melting points of these compounds in degrees Kelvin can be estimated by the equation:

$$TM = 59.9*(SIGMAL) + 12.9*(SUMDM) + 430.2*(ALPHAL) + 64.8*(PACK1) + 50.8*(PACK8) + 32.5*(SYM9) - 292.4 \quad (5)$$

n = 124 r = 0.976 std. dev = 19.2

The second regression analysis extends the first analysis by now including nitro, cyano, and fluoro benzenes to the original data set. This multiple regression analysis model contains TM, melting point of the compound in Kelvin, as the dependent variable and the same independent variables as equation 5. A summary of the regression analysis is contained in Table 5. The melting points of these compounds can be estimated by the equation:

$$TM = 57.1*(SIGMAL) + 11.5*(SUMDM) + 419.0*(ALPHAL) + 50.0*(PACK1) + 48.1*(PACK8) + 17.2*(SYM9) - 265.9 \quad (6)$$

n = 275 r = 0.916 std. dev = 29.2

The third regression analysis contains 490 non-hydrogen bonding aromatic compounds. This data set includes the benzene derivatives found in the previous data set and polycyclic aromatic hydrocarbons such as phenanthrenes, naphthalenes and biphenyls. Substituents on these aromatic molecules include halogen, methyl, cyano and nitro groups. A summary of the regression analysis is contained in Table 5. The melting points, of these aromatic compounds can be estimated by the equation:

$$TM = 11.6*(EXPAN) + 104.0*(SIGMAL) + 10.5*(SUMDM) + 384.2*(ALPHAL) - -20.7*(CBRBIPH) + 12.0*(CBR) - 259.9 \quad (7)$$

n = 490 r = 0.893 std. dev = 36.3

It is important to note that the parameter estimates for SUMDM and ALPHAL are nearly constant in the three regression analyses. The values of SIGMAL, PACK1, PACK8 and PACK9 are also nearly constant when used in the first two regression analyses.

HYDROGEN BONDING AND NON HYDROGEN BONDING COMPOUNDS

A generalized equation has been developed for estimating the melting points of rigid, hydrogen bonding and non-hydrogen bonding aromatic compounds. These compounds include benzene derivatives, polycyclic compounds and biphenyl derivatives. The equation developed includes both additive constitutive and non-additive non-constitutive properties of the molecules.

The variables CBR, CBRBIPH, CH3, F, CL, BR, I, NO2, CHO, OCH3, COOH, OH, NH2, CONH2 and CN are all indicator variables that help to describe the additive constitutive contributions all of these groups have to the melting point of these aromatic compounds. All of these variables have a positive influence on the melting point except for fluorine which is negative. A summation of the additive contribution of these groups to the melting point of a compound leads to a total melting point number (TMPN).

$$TMPN = \sum n_i \, MPN_i \qquad (8)$$

where n_i is the number of times each functional group of type i appears in the molecule, and MPN is the melting point number for each functional group in the molecule. The melting point numbers for all of the functional groups in the analysis are given in Table 6.

The variables COOH_COOH, COOH_CONH, COOH_NH2, COOH_X, COO_OH, COOH_NO2, COOH_CHO, OH_OH, OH_NO2, OH_CHO and NH2_NH2 are all used to form an intramolecular hydrogen bonding number (IHBN). Compounds that are capable of forming an intramolecular hydrogen bond will melt at a much lower temperature than their isomers which form intermolecular hydrogen bonding. Those hydrogen bonds that are entirely tied up by intramolecular interactions are not available for interaction with neighboring molecules. They therefore do not contribute to an increase in the melting point number. From the above reasoning, the IHBN of such a hydrogen bond interaction should always be negative. Table 7 lists the IHBN for all of the hydrogen bond interactions that were found significant in this study. All of the values in table 7 are negative, which confirms the theory. COOH_COOH refers

to an ortho dicarboxylic acid. COOH_X refers to any halogen that is ortho to a carboxylic acid group. The rest of the variables in table 7 are self explanatory. Other possible hydrogen bonding interactions were also tested for statistical significance. For example OH_NH2 and NH2_CHO interactions were tested, but found not to be significant. Since it is possible for a molecule to have more than one pair of intramolecular hydrogen bonding groups in a molecule, the total intramolecular hydrogen bonding number (TIHBN) of a molecule will be a summation of all such interactions.

$$TIHBN = \sum n_i IHBN_i \qquad (9)$$

SIGMAL is the logarithm of the rotational symmetry number of the molecule. The rotational symmetry number is defined as the number of orientations of the molecule indistinguishable from a reference position. All groups are treated as symmetrical in this framework. In calculating the symmetry number of a molecule, the following groups are considered to be equal in size:

methyl = chloro = bromo = cyano (10)

iodine = amide (11)

hydroxyl = amino (12)

fluoro = hydrogen (13)

The justification for using this system of equal size for the groups above is based on the positional disordering of rigid molecules. It is possible for a molecule without a center of symmetry to form centrosymmetric crystals. The space lattice of such crystals will have an equal number of points facing in opposite directions. Disordered rigid crystals such as these can be formed only when both crystal arrangements have similar energy. For example p-chlorobromobenzene and p-nitrochlorobenzene have been found through x-ray diffraction analysis to form such crystals. From an intuitive point of view, molecular symmetry is a measure of the probability that a freely rotating molecule will be oriented in a manner suitable for incorporation into the crystal. This definition of SIGMAL could help explain the positional disordering of crystals.

In order to understand the symmetry behavior of biphenyl derivatives, two different approaches were used. In treating biphenyl compounds, it is clear that the aromatic rings may

not be planar. The first approach treats the biphenyl compounds as rigid and planar. The second approach treats the two rings in a biphenyl molecule as non-planar. A non-planar biphenyl derivative will have a symmetry number that is one-half the value expected for the compound if it were planar. From statistical analysis of the data it was found that the first approach, considering the aromatic rings as planar, gave a better correlation than treating the rings as non-planar.

The variables PACK1, PACK8 , PACK9, PACK10 and PACK11 are indicator variables to indicate various structural features of the molecule. Thirteen different structural features such as meta-, ortho- and para- substituted benzenes were tested. From statistical analysis, five of these indicator variables were found to be significant. PACK1 refers to any hexa-substituted benzene molecule such as hexabromobenzene or 1,2,3-trichloro-4,5,6-triiodobenzene. PACK8 is any para-substituted benzene molecule while PACK9 refers to a 1,2,4,5-tetrasubstituted benzene compound. PACK10 indicates a 1,2,4-trisubstituted benzene molecule while PACK11 indicates a 1,2,3-trisubstituted benzene derivative. These indicator variables can be thought of as factors that influence the enthalpy of melting by increasing the packing efficiency of the crystal, which decreases the separation distance between interacting groups of complex molecules. Table 8 lists the packing efficiency index (TPACK) for all of the indicator variables discussed above.

EXPAN which is the eccentricity of the molecule to the third power, can be related to the difference in packing efficiency between the liquid and the crystal. The greater the eccentricity of a molecule, the greater the increase in volume required for the rotational freedom that occurs on melting.

$$\text{EXPAN} = \frac{\text{volume required for complete free rotation}}{\text{volume occupied by the molecule}} \qquad (14)$$

Therefore, EXPAN is very important for polycyclic molecules.

A generalized equation for the estimation of the melting point of a wide variety of both hydrogen bonding and non-hydrogen bonding aromatic compounds can now be given:

$$\text{TM} = \text{TMPN} + \text{TIHBN} + \text{TPACK} + 8.89*\text{EXPAN} + 73.1*\text{SIGMAL} + 196.3 \qquad (15)$$

n = 1228 std. dev. = 34.7 r = 0.892

TM is the melting point of the compound in Kelvin. TMPN is the total melting point number for the molecule as previously discussed. The melting point numbers for all of the functional groups in the analysis are given in Table 6. TIHBN is the total intramolecular hydrogen bonding index. The values for IHBN appear in Table 7. TPACK is the packing efficiency index for the molecule. The values for TPACK appear in Table 8. EXPAN is the eccentricity of the molecule taken to the third power and SIGMAL is the log symmetry number for the molecule. Table 9 gives a summary of the multiple regression analysis. To illustrate the use of equation 15, two examples are worked-out in Appendix E.

FLEXIBLE COMPOUNDS

Molecular flexibility and rotational symmetry were used to develop an empirical equation for predicting the entropy of fusion for non-rigid organic molecules. The equation was applied to a series of alkanes of varying degree of flexibility. The heats of fusion for these compounds were estimated from additive constitutive properties. The melting point, TM, is given by

$$TM = \frac{\triangle H_f}{\triangle S_f} \qquad (16)$$

where $\triangle H_f$ and $\triangle S_f$ refer to enthalpy and entropy of fusion respectively. The equations developed for $\triangle H_f$ and $\triangle S_f$ were successfully used to estimate the melting points of these compounds.

The enthalpy of fusion of the aliphatic paraffins can be estimated from the following equation:

$$\triangle H_f = 328.4\ (CH) + 800.9\ (CH_2) + 283.9\ (CH_3) - 1070.0$$

$$r = 0.948 \qquad \text{std.dev.} = 769.3\ \text{cal}/^{\circ}\text{K mol} \qquad n = 145 \qquad (17)$$

The variables CH_3, CH_2, and CH represent the number of methyl, methylene and CH groups in the molecule respectively. It is important to notice that a fourth variable, which accounts for the tertiary carbons in the molecule, is not necessary since the intercept of the above equation essentially accounts for these carbons. Equation 17 enables us to predict the enthalpy of fusion of these compounds from additive constitutive properties. A summary of the regression analysis is contained in Table 10. All of the parameters in the equation are statistically significant. This can be seen from an evaluation of the T-test values. The number of methyl and CH groups in the molecule are somewhat

collinear since each branch adds a methyl group in addition to a CH group or a tetrasubstituted carbon. Therefore the coefficients of CH_3 and CH cannot be evaluated independently for this dataset.

In order to estimate the entropy of fusion of a flexible molecule, one has to be able to quantify its internal entropy of fusion, ΔS_{int}, which is the measure of the conformational freedom of the molecule. In the solid phase flexible molecules are thought to have a regular crystalline structure with the molecules in a fully outstretched position and aligned parallel to one another. On the contrary in the liquid phase, molecules are not only free in their position and orientation but are also free in their conformation. They may be fully outstretched or coiled to some extent. In order to estimate the probability of finding a fully outstretched liquid molecule, we need to account for the number of energetically reasonable conformations possible for a molecule in the liquid. Further, this number must account not only for a straight chain of n-carbons but also for any branches that originate in the chain.

Molecular Flexibility: A long chain of n carbon atoms will have n-1 carbon-carbon bonds, n-2 C-C-C bond angles and n-3 C-C-C-C dihydral angles. Melting has little effect on bond lengths and bond angles, but it significantly affects the dihydral angles. In the crystal, all dihydral angles in the molecule are 180°(anti-conformation), that is, the bulky alkyl groups on each carbon are as far apart as they can be. In the liquid, there are two additional conformations that are likely to be observed (8). These are the two gauche conformations in which the alkyl groups are only 60° apart. The latter are mirror images of each other and are of the same stability; nevertheless they are distinct.

If we assume that the three conformations are equally probable, then the total number of distinct and energetically possible arrangements, that a straight chain molecule can have in the liquid is

$$\phi = 3^{(n-3)} \quad (18)$$

where (n-3) is the number of dihydral angles in the chain. We define ϕ as the molecular flexibilty number. However, most flexible molecules or molecular fragments we encounter in applied chemistry contain one or more branches. When branching occurs equation (18) becomes

$$\phi = 3^{(n-3-B-T)} \quad (19)$$

where n is the total number of carbons, B is the total number

of branches and T is the number of t-butyl groups in the molecule. The flexibility number of n-pentane is 9 and that of 2-ethyl pentane is 27. The addition of a flexible branch increases the flexibility of a molecule. Addition of nonflexible branching to the molecule on the other hand, has no effect on the flexibility of the latter, unless it results in the formation of t-butyl groups. The methyl groups of a t-butyl fragment are small enough to be considered as three equivalent fast rotating spheres that favor no particular conformation . The flexibility numbers of 2-methylpentane and 2,2-dimethylpentane are 9 and 3 respectively. Similarly the rigid compounds 2,2,4,4-tetramethylpentane and 2,2,3,3,4,4-hexamethylpentane have a ϕ value of unity.

Since ϕ represents the total ensemble of arrangements in the liquid, the probability of finding a fully outstretched flexible molecule in the liquid is $1/\phi$. We can thus express the internal entropy of fusion of flexible molecules in terms of the flexibility number ϕ as follows:

$$\Delta S_{int} = 4.6 \log(\phi) \qquad (20)$$

The following regression analysis describes the estimation of the entropy of fusion of aliphatic paraffins, from non-additive non-constitutive properties of the molecules i.e.

$$\Delta S_f = 7.5 + 5.1 \log(\phi) - 0.6 \text{ SIGMAL}$$

$$r = 0.920 \quad \text{std.dev.} = 4.1 \text{ cal}/^{o}\text{K mol} \quad n = 72 \qquad (21)$$

The rotational entropy of melting is determined from the logarithm of the rotational symmetry, and the conformational entropy is described in terms of the molecular flexibility. A summary of this regression is contained in Table 11. The T - test value for rotational entropy is low, suggesting low statistical significance for this parameter. This is probably due to two reasons. First this dataset contains a significant number of n-paraffins, which all have the same SIGMA value of 2 and since the flexibility of these compounds increases constantly with increasing number of carbons in the chain, ϕ is sufficient in expressing the melting entropies of the n-paraffins. Second, the branched compounds do not have substantially different rotational symmetries. As a result the statistical weight of rotational symmetry for the entire dataset is diminished. The intent of this regression however, is not to provide a dataset basis for testing the dependence of rotational entropy on rotational symmetry. We use the concept here in order to complete the quantitative description of the entropy of fusion.

The estimated coefficient of the logarithm of the molecular flexibility in equation 21 shows excellent agreement with the theoretically expected value from equation 20.

Having estimated the enthalpy and the entropy of fusion of aliphatic paraffins we can now attempt to predict their melting points. The latter can be calculated from equation 16. We can use equation 17 for ΔH_f and equation 21 for ΔS_f. The calculated TM is thus

$$TM_{calc} = \frac{328.4\ (CH) + 800.9\ (CH_2) + 283.9\ (CH_3) - 1070.0}{7.5 + 5.1 \log(\phi) - 0.6\ SIGMAL} \qquad (22)$$

and the linear regression analysis of the observed versus the calculated melting points gives the following results:

$$TM_{obs} = 5.4 + TM_{calc}$$

$$r = 0.888 \qquad \text{std.dev.} = 38.2^{\circ}K \qquad n=102 \qquad (23)$$

Considering the fact that the dataset provides a melting point range of $300^{\circ}K$ the results of equation 23 can be conservatively characterised as acceptable. The reason for the relatively low r value is not clear. One possibility may be the fact that the measurement of the enthalpy and the entropy of fusion is generally subject to significant experimental error. If this is the case, then theobserved values for ΔH_f and ΔS_f may alter the calculated r value in one or the other direction. To avoid such a problem, one can use the coefficients of equations 17 and 21 as parameter estimates in a non-linear correlation. Then the observed enthalpy and entropy values are used as approximate values and the regression rigorously depends only on the observed melting points, which can be measured fairly accurately and with little error. The reason a non-linear model is necessary in this case is because an equation that has the following form

$$TM = \frac{a + b\ (CH) + c\ (CH_2) + d\ (CH_3)}{d + e \log(\phi) + f\ SIGMAL} \qquad (24)$$

is a non-linear equation.

We performed the non-linear regression and the equation obtained is the following:

$$TM = \frac{370.8\ (CH) + 1188.7\ (CH_2) + 944.6\ (CH_3) - 817.4}{31.9 + 5.8 \log(\phi) - 11.4\ SIGMAL}$$

$$r = 0.972 \qquad \text{sdt.dev.} = 19.5K^{o} \qquad n = 102 \qquad (25)$$

The coefficient of the logarithm of the flexibility function in equation 25 is very good and the r value is drastically improved in comparison to the linear model. Also, the convergence temperature predicted by equation 25 is 429°K, which compares reasonably well with the 419°K previously reported for n-paraffins in the literature (9). Two examples in using equation 25 are provided in Appendix F.

In conclusion, one simple equation (Equation 15) has been developed that can estimate the melting point of a wide variety of rigid organic compounds and one equation (Equation 25) that can estimate the melting point of flexible molecules. The two equations utilize both additive and non-additive properties of molecules.

BIBLIOGRAPHY

(1) S.H. Yalkowsky and S.C. Valvani, J. Pharm. Sci. 69: 912 (1980)

(2) S.H. Yalkowsky and S.C. Valvani, J. Chem. Eng. Data, 24: 127 (1979)

(3) Merck Index, Ninth Edition, ed: M. Windholz, Merck & Co., Inc., Rahway, NJ (1976)

(4) Handbook of Chemistry and Physics, 1973-1974. 54th Ed. CRC Press, Boca Raton, FL (1972)

(5) Handbook of American Petroleum Institute Project 44, ed: Texas A&M University System, College Station, TX (1984)

(6) L.N. Ferguson, The Modern Structural Theory of Organic Chemistry. Prentice-Hall (1963)

(7) J.T. Edward, "Molecular Volumes and the Stokes Einstein Equation.", J. Chem. Educ., 47(4):261-270 (1970)

(8) A. I. Kitaigorodsky, Molecular Crystals and Molecules, ed: Academic Press Inc., New York, NY (1973)

(9) H.L. Bhatnagar and S. Aggarwal, J. Indian Chem. Soc., 56: 96-98 (1979)

(10) C.P. Smyth, Dielectric Behavior and Structure. McGraw-Hill, New York, NY (1955)

TABLE 1. GROUP CONTRIBUTIONS TO DIPOLE MOMENTS

Functional Group	Dipole Moment[a] (Debyes)
F	1.43
Cl	1.55
Br	1.52
I	1.30
CN	3.90
CH_3	0.40
OH	1.60
OCH_3	1.25
COOH	1.64
NH_2	1.53
NO_2	3.98
$COCH_3$	2.89
CH_2OH	1.68
C_2H_5	0.40
NCO	2.32

[a]source:Smyth (1955), Reference 10.

TABLE 2. GROUP CONTRIBUTIONS TO POLARIZABILITY

Functional Group	Polarizability[a] (angstrom^3)
F	0.38
Cl	2.28
Br	3.34
I	5.11
CN	2.12
H	0.42
C	0.93
CH_2	1.77
O(hydroxyl)	0.59
O(ether)	0.64
O(carbonyl)	0.84
Double bond	0.58 extra
Triple bond	0.86 extra
N(primary)	0.87
N(secondary)	0.93
N(tertiary)	1.03
C_6H_5	9.38

[a]source:Ferguson (1963)

TABLE 3. GROUP CONTRIBUTIONS TO VAN DER WAALS VOLUME

Functional Group	Volume[a] (A^3)
C (single bond)	5.6
C (double bond)	8.1
C (triple bond)	13.4
H (attached to C)	5.3
H (attached to aromatic C)	5.2
H (attached to N)	5.2
H (attached to O)	7.2
F	9.9
Cl	19.8
Br	24.5
I	32.8
O (ether)	6.2
O (double bond)	11.3
N (single bond)	7.2
N (double bond)	8.6
N (triple bond)	11.0
NO_2	27.9

[a]source: Edward (1970)

TABLE 4. VARIABLES USED IN MULTIPLE REGRESSION ANALYSES

Variable	Definition
TM	Melting point of the compound in Kelvin
ALPHAL	Logarithm of the polarizability as calculated fromthe group values of Ferguson
SUMDM	The summation of the group dipole moments of the molecule
PACK1	A hexa-substituted benzene molecule
PACK8	A para compound
PACK9	A 1,2,4,5-tetrasubstituted benzene molecule
EXPAN	The eccentricity of the molecule taken to the third power
SIGMAL	The logarithm of the symmetry number for the molecule.
CBR	The number of bridgehead carbon atoms in a molecule
CBRBIPH	The number of carbon atoms in a molecule that are involved in a biphenyl linkage.

TABLE 5. SUMMARY OF REGRESSION ANALYSES FOR EQUATIONS 5,6,7

A. SIX PARAMETER EQUATION
INCLUDES CHLORO, BROMO, IODO, AND METHYL SUBSTITUTED BENZENE DERIVATIVES

PARAMETER	ESTIMATE	T	SIG	N	STD DEV	R
INTERCEPT	-292.4	-10.4	0.0001	124	19.17	0.977
SIGMAL	59.9	6.2	0.0001			
SUMDM	12.9	10.4	0.0001			
ALPHAL	430.2	17.8	0.0001			
PACK1	64.8	6.7	0.0001			
PACK8	50.8	7.2	0.0001			
PACK9	32.5	4.6	0.0001			

B. SIX PARAMETER EQUATION
INCLUDES FLUORO, CHLORO, BROMO, IODO, METHYL, NITRO AND CYANO SUBSTITUTED BENZENE DERIVATIVES

PARAMETER	ESTIMATE	T	SIG	N	STD DEV	R
INTERCEPT	-265.9	-10.2	0.0001	275	29.2	.916
SIGMAL	57.1	7.1	0.0001			
SUMDM	11.5	16.8	0.0001			
ALPHAL	419.0	19.6	0.0001			
PACK1	50.0	5.3	0.0001			
PACK8	48.1	7.2	0.0001			
PACK9	17.1	2.4	0.0189			

C. SIX PARAMETER EQUATION
INCLUDES FLUORO, CHLORO, BROMO, IODO, METHYL, NITRO AND CYANO SUBSTITUTED AROMATIC COMPOUNDS

PARAMETER	ESTIMATE	T	SIG	N	STD DEV	R
INTERCEPT	-259.9	-9.3	0.0001	490	36.3	.893
SIGMAL	104.0	17.5	0.0001			
SUMDM	10.5	17.5	0.0001			
ALPHAL	384.2	16.7	0.0001			
EXPAN	11.6	6.4	0.0001			
CBRBIPH	-20.7	-6.5	0.0001			
CBR	12.0	8.0	0.0001			

.pa

TABLE 6. MELTING POINT NUMBERS FOR FUNCTIONAL GROUPS

Functional Group		MPN
CH3	(Methyl)	7.54
F	(Fluorine)	-14.20
CL	(Chlorine)	21.39
BR	(Bromine)	30.66
I	(Iodine)	42.81
NO2	(Nitro)	53.78
CHO	(Aldehyde)	50.37
OCH3	(Methoxy)	14.79
COOH	(Carboxy)	150.60
OH	(Hydroxyl)	68.73
NH2	(Amino)	56.03
CONH2	(Amide)	134.69
CN	(Cyano)	53.27

TABLE 7. INTRAMOLECULAR HYDROGEN BOND INDEX

Intramolecular Hydrogen Bond	IHBN
COOH_COOH	-122.2
COOH_NH2	-20.3
COOH_X	-17.4
COOH_CONH2	not determined
COOH_OH	-71.5
COOH_NO2	-19.9
COOH_CHO	-55.6
OH_OH	-44.0
OH_NO2	-33.7
OH_CHO	-37.9
NH2_NH2	-12.0

TABLE 8. PACKING EFFICIENCY INDEX

Variable	TPACK
PACK1	73.4
PACK8	9.5
PACK9	24.0
PACK10	14.5
PACK11	11.7

TABLE 9. SUMMARY OF REGRESSION ANALYSIS FOR EQUATION 15

PARAMETER	ESTIMATE	T	SIG	N	STD. DEV	R
INTERCEP	196.3438	35.075	0.0001	1229	34.7	0.892
CBR	29.71545	31.698	0.0001			
CBRBIPH	16.21747	7.870	0.0001			
CH3	7.539882	5.111	0.0001			
F	-14.1963	-4.037	0.0001			
CL	21.38803	18.252	0.0001			
BR	30.66166	17.961	0.0001			
I	42.80789	20.046	0.0001			
NO2	53.77544	29.790	0.0001			
CHO	50.36379	12.194	0.0001			
OCH3	14.79027	5.768	0.0001			
COOH	150.6002	39.311	0.0001			
OH	68.72652	26.728	0.0001			
NH2	56.03248	22.642	0.0001			
CONH	134.6926	17.165	0.0001			
CN	53.26742	9.146	0.0001			
COOHCOOH	-122.184	-20.562	0.0001			
COOH_NH2	-20.3257	-1.894	0.0585			
COOH_X	-17.3489	-3.117	0.0019			
COOH_OH	-71.5464	-5.914	0.0001			
COOH_NO2	-19.9149	-2.142	0.0324			
COOH_CHO	-55.5655	-1.584	0.1134			
OH_OH	-43.9565	-8.701	0.0001			
OH_NO2	-33.6572	-5.767	0.0001			
OH_CHO	-37.9098	-4.482	0.0001			
NH2_NH2	-12.016	-1.729	0.0840			
EXPAN	8.892498	7.882	0.0001			
PACK1	73.42496	10.100	0.0001			
PACK8	9.457965	1.940	0.0526			
PACK9	23.95851	4.242	0.0001			
PACK10	14.48447	3.637	0.0003			
PACK11	11.7184	3.953	0.0001			
SIGMAL	73.12523	13.218	0.0001			

TABLE 10. SUMMARY OF ENTHALPY OF FUSION REGRESSION ANALYSIS

PARAMETER	ESTIMATE	T	PROB > |T|	N	STD.DEV.	R
INTERCEPT	-1070.0	-2.8	0.0067	145	769.3	0.948
CH	328.4	4.6	0.0001			
CH_2	800.9	28.2	0.0001			
CH_3	283.9	4.0	0.0001			

TABLE 11. SUMMARY OF ENTROPY OF FUSION REGRESSION ANALYSIS

PARAMETER	ESTIMATE	T	PROB > |T|	N	STD.DEV.	R
INTERCEPT	7.5	9.9	0.0001	72	4.1	0.920
log (ϕ)	5.1	19.1	0.0001			
log (σ)	-0.6	-0.2	0.8397			

APPENDIX A

dBASE III PROGRAM TO CALCULATE MOLECULAR PARAMETERS

```
USE HEMP2
GOTO 1
DO WHILE .NOT. EOF()
STORE CHAR*13.4 + CAR*8.1 + CBR*8.1 + C*5.6 + CH*11.3+;
      CH2*17.0 + CH3*22.7 + F*9.9 + CL*19.8 + BR*24.5+;
      I*32.8 + NO2*27.9 + CHO*25.1 + OH*13.4 + COOH*32.8+;
      CONH*37.0 + O*6.2 + NH2*17.6 + NHCO*31.8 + COO*25.6+;
      DOUBLE*5.0+TRIPLE*10.6+CBRBIPH*8.1+CBRRIG*8.1+CH2RIGID*19.5+;
      CN*24.4 TO X1
STORE CHAR*13.0 + CAR*12.0 + CBR*12.0 + C*12.0 + CH*13.0+;
      CH2*14.0 + CH3*15.0 + F*19. + CL*35.5 + BR*79.9+;
      I*126.9 + NO2*46.0 + CHO*29.0 + OH*17.0 + COOH*45.0+;
      CONH*44.03 +  O*16.0 + NH2*16.0 + NHCO*43.0 + COO*44.0+;
      CBRBIPH*12.+CBRRIG*12.+CH2RIGID*14.+CN*26.0 TO Y1
      CHAR*1.64 + CAR*1.22 + CBR*1.22 + C*0.93 + CH*1.35+;
      CH2*1.77 + CH3*2.19 + F*0.38 + CL*2.28 + BR*3.34+;
      I*5.11 + NO2*2.51 + CHO*2.19 + OH*1.01 + COOH*2.78+;
      CONH*3.48 + O*0.64 + NH2*1.71 + NHCO*3.12 + COO*2.36+;
      DOUBLE*.58+TRIPLE*0.86+CBRBIPH*1.22+CBRRIG*1.22+;
      CH2RIGID*1.77+CN*2.12 TO X2
STORE CH3*0.4 + F*1.46 + CL*1.58 + BR*1.54+;
      I*1.30 + NO2*3.98 + CHO*2.76+ OH*1.60 + COOH*1.64+;
      CONH*3.62 + O*1.25 + NH2*1.53 + NHCO*3.20 + COO*1.83+;
      DOUBLE*0.4+TRIPLE*0.7+CH2RIGID*.4+CN*3.9 TO X8
STORE CHAR*.35 + CAR*.13 + CBR*.22 + C*.2 + CH*.43+;
      CH2*.66 + CH3*.89 + F*0.37 + CL*0.94 + BR*1.09+;
      I*1.35 - NO2*0.03 - CHO*0.42- OH*0.44 - COOH*0.03+;
      0.0 - CONH*1.58 - O*0.61 - NH2*1.00 - NHCO*0.87 - COO*0.56+;
      0.0-DOUBLE*.55-TRIPLE*1.42+CBRBIPH*.13+CBRRIG*.22+;
      CH2RIGID*.66-CN*0.34 TO L
REPLACE VOLUME WITH X1
REPLACE ALPHA WITH X2
REPLACE SUMDM WITH  X8
REPLACE MW WITH Y1
REPLACE LOGPC WITH L
SKIP
ENDDO
CLEAR
```

APPENDIX B

EXPERIMENTAL DATA FOR RIGID ORGANIC COMPOUNDS

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
O-FLUOROMETHYLBENZENE	110.0	-62.0	8.09	102.40	11.57	1.86	2
P-FLUOROMETHYLBENZENE	110.0	-56.8	8.88	102.40	11.57	1.86	2
O-FLUOROANILINE	111.0	-28.5	8.00	97.30	11.09	2.99	1
P-FLUOROANILINE	111.0	-0.8	8.40	97.30	11.09	2.99	2
CHLOROBENZENE	112.5	-50.0	8.15	94.90	11.70	1.58	2
M-DIFLUOROBENZENE	114.0	-59.0	7.85	89.60	9.76	2.92	12
O-DIFLUOROBENZENE	114.0	-34.0	7.85	89.60	9.76	2.92	12
P-DIFLUOROBENZENE	114.0	-13	8.61	89.60	9.76	2.92	12
2-METHYLBENZONITRILE	117.0	-13.5	8.92	116.90	13.81	4.30	2
3-METHYLBENZONITRILE	117.0	-23.0	9.28	116.90	13.81	4.30	2
4-METHYLBENZONITRILE	117.0	29.5	9.89	116.90	13.81	4.30	4
2-AMINO-BENZONITRILE	118.0	51.0	8.94	111.80	13.33	5.43	1
3-AMINO-BENZONITRILE	118.0	53.0	9.27	111.80	13.33	5.43	1
4-AMINO-BENZONITRILE	118.0	86.0	9.75	111.80	13.33	5.43	2
INDAN	118.0	-51.4	9.05	120.80	14.31	0.00	1
2-HYDROXYBENZONITRILE	119.0	98.0	8.84	107.60	12.63	5.50	1
3-HYDROXYBENZONITRILE	119.0	83.0	9.27	107.60	12.63	5.50	1
4-HYDROXYBENZONITRILE	119.0	113.0	9.72	107.60	12.63	5.50	2
5-AMINO-1,4-DIHYDRONAPHTHALENE	119.0	37.5	9.95	116.10	13.83	1.53	1
1,2,3-TRIMETHYLBENZENE	120.0	-25.5	8.96	132.60	15.15	1.20	2
1,2,4-TRIMETHYLBENZENE	120.0	-43.8	9.08	132.60	15.15	1.20	1
1,3,5-TRIMETHYLBENZENE	120.0	-52.7	8.96	132.60	15.15	1.20	6
1-METHYLETHYLBENZENE(CUMENE)	120.0	-96.0		131.80	15.15	0.80	1
PROPYLBENZENE	120.0	-99.2		131.80	15.15	0.40	1
2,4-DIMETHYLANILINE	121.0	-14.3	9.01	127.50	14.67	2.33	1
2,5-DIMETHYLANILINE	121.0	15.5	9.10	127.50	14.67	2.33	1
2,6-DIMETHYLANILINE	121.0	11.2	9.00	127.50	14.67	2.33	2
2-AMINOBENZALDEHYDE	121.0	39.0	8.59	112.50	12.90	4.29	1
3,4-DIMETHYLANILINE	121.0	51.0	8.90	127.50	14.67	2.33	1
3,5-DIMETHYLANILINE	121.0	9.8	8.07	127.50	14.67	2.33	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
BENZENE	78.0	5.5	7.07	80.40	9.84	0.00	12
TOLUENE	92.0	-95.0	8.09	97.80	11.61	0.40	2
ANILINE	93.0	-6.3	8.04	92.70	11.13	1.53	2
PHENOL	94.0	43.0	7.98	88.50	10.43	1.60	2
FLUOROBENZENE	96.0	-41.0	7.85	85.00	9.80	1.46	12
PHENYLACETYLENE	102.0	-44.8	9.91	107.60	12.56	0.70	2
BENZONITRILE	103.0	-13.0	8.89	99.50	12.04	3.90	2
STYRENE	104.0	-33.0	9.55	108.40	13.12	0.40	1
BENZALDEHYDE	106.0	-26.0	9.74	100.20	11.61	2.76	2
ETHYLBENZENE	106.0	-50.0	9.30	114.80	13.38	0.40	1
M-XYLENE	106.0	-47.0	8.96	115.20	13.38	0.80	2
O-XYLENE	106.0	-25.0	8.09	115.20	13.38	0.80	2
P-XYLENE	106.0	13.0	9.08	115.20	13.38	0.80	4
2-AMINOTOLUENE	107.0	-27.7	8.09	110.10	12.90	1.93	1
3-AMINOTOLUENE	107.0	-30.4	8.09	110.10	12.90	1.93	1
4-AMINOTOLUENE	107.0	43.5	9.03	110.10	12.90	1.93	2
1,2-DIAMINOBENZENE	108.0	102.0	7.95	105.00	12.42	3.06	2
1,3-DIAMINOBENZENE	108.0	63.0	8.69	105.00	12.42	3.06	2
1,4-DIAMINOBENZENE	108.0	140.0	8.87	105.00	12.42	3.06	4
2-HYDROXYTOLUENE	108.0	30.0	8.09	105.90	12.20	2.00	1
3-HYDROXYTOLUENE	108.0	11.1	8.74	105.90	12.20	2.00	1
4-HYDROXYTOLUENE	108.0	34.8	8.93	105.90	12.20	2.00	2
ANISOLE	108.0	-37.5	9.32	104.00	12.25	1.65	2
2-AMINOPHENOL	109.0	174.0	8.04	100.80	11.72	3.13	2
3-AMINOPHENOL	109.0	123.0	8.67	100.80	11.72	3.13	2
4-AMINOPHENOL	109.0	186.0	8.87	100.80	11.72	3.13	4
1,2-DIHYDROXYBENZENE	110.0	105.0	7.98	96.60	11.02	3.20	2
1,3-DIHYDROXYBENZENE	110.0	111.0	8.59	96.60	11.02	3.20	2
1,4-DIHYDROXYBENZENE	110.0	170.0	8.84	96.60	11.02	3.20	4
M-FLUOROMETHYLBENZENE	110.0	-87.7	8.40	102.40	11.57	1.86	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
3-AMINOBENZALDEHYDE	121.0	28.0	9.25	112.50	12.90	4.29	1
4-AMINOBENZALDEHYDE	121.0	71.0	9.50	112.50	12.90	4.29	2
4-FLUOROBENZONITRILE	121.0	34.8	9.31	104.10	12.00	5.36	2
BENZAMIDE	121.0	132.0	9.35	112.10	12.90	3.62	2
2,3-DIAMINOTOLUENE	122.0	63.0	8.09	122.40	14.19	3.46	1
2,4-DIAMINOTOLUENE	122.0	99.0	9.03	122.40	14.19	3.46	1
2,5-DIAMINOTOLUENE	122.0	64.0	8.77	122.40	14.19	3.46	1
2,6-DIAMINOTOLUENE	122.0	106.0	8.69	122.40	14.19	3.46	2
2-HYDROXYBENZALDEHYDE	122.0	-7.0	8.52	108.30	12.20	4.36	1
3,4-DIAMINOTOLUENE	122.0	88.5	9.03	122.40	14.19	3.46	1
3-HYDROXYBENZALDEHYDE	122.0	106.0	9.20	108.30	12.20	4.36	1
4-HYDROXYBENZALDEHYDE	122.0	116.0	9.47	108.30	12.20	4.36	2
BENZOIC ACID	122.0	122.4	9.31	107.90	12.20	1.64	2
1,2,3-TRIAMINOBENZENE	123.0	103.0	8.69	117.30	13.71	4.59	2
1,2,4-TRIAMINOBENZENE	123.0	98.0	8.87	117.30	13.71	4.59	1
2-AMINO-3-HYDROXYTOLUENE	123.0	148.0	8.74	118.20	13.49	3.53	1
2-AMINO-4-HYDROXYTOLUENE	123.0	157.0	8.93	118.20	13.49	3.53	1
2-AMINO-5-HYDROYTOLUENE	123.0	179.0	8.87	118.20	13.49	3.53	1
2-AMINO-6-HYDROXYTOLUENE	123.0	129.0	8.67	118.20	13.49	3.53	2
3-AMINO-2-HYDROXYTOLUENE	123.0	89.0	8.77	118.20	13.49	3.53	1
3-AMINO-4-HYDROXYTOLUENE	123.0	137.0	8.93	118.20	13.49	3.53	1
3-AMINO-5-HYDROXYTOLUENE	123.0	139.0	8.77	118.20	13.49	3.53	2
4-AMINO-3-HYDROXYTOLUENE(DEC)	123.0	162.0	9.03	118.20	13.49	3.53	1
5-AMINO-2-HYDROXYTOLUENE	123.0	175.0	8.87	118.20	13.49	3.53	1
M-METHOXYANILINE	123.0	-1.0	9.20	116.30	13.54	3.18	1
NITROBENZENE	123.0	5.7	8.35	103.00	11.93	3.98	2
O-METHOXYANILINE	123.0	6.2	9.20	116.30	13.54	3.18	1
P-METHOXYANILINE	123.0	57.2	10.18	116.30	13.54	3.18	2
2,3-DIHYDROXYTOLUENE	124.0	68.0	8.74	114.00	12.79	3.60	1
2,4-DIHYDROXYTOLUENE	124.0	105.0	8.93	114.00	12.79	3.60	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,5-DIHYDROXYTOLUENE	124.0	124.0	8.84	114.00	12.79	3.60	1
3,4-DIHYDROXYTOLUENE	124.0	65.0	8.93	114.00	12.79	3.60	1
3,5-DIHYDROXYTOLUENE	124.0	107.0	8.74	114.00	12.79	3.60	2
3,5-DIHYDROXYANILINE	125.0	146.0	8.10	108.90	12.31	4.73	6
1,2,3-TRIHYDROXYBENZENE	126.0	132.8	8.59	104.70	11.61	4.80	2
1,2,4-TRIHYDROXYBENZENE	126.0	140.5	8.84	104.70	11.61	4.80	1
1,3,5-TRIHYDROXYBENZENE	126.0	217.0	8.59	104.70	11.61	4.80	6
1-FLUORO-2-METHOXYBENZENE	126.0	-39.0	9.32	108.60	12.21	3.11	2
1-FLUORO-4-METHOXYBENZENE	126.0	-45.0	9.84	108.60	12.21	3.11	2
M-METHYLCHLOROBENZENE	126.5	-47.8	8.70	112.30	13.47	1.98	2
O-METHYLCHLOROBENZENE	126.5	-35.1	8.15	112.30	13.47	1.98	2
P-METHYLCHLOROBENZENE	126.5	7.5	9.18	112.30	13.47	1.98	4
M-CHLOROANILINE	127.5	-10.3	8.50	107.20	12.99	3.11	1
O-CHLOROANILINE	127.5	-14.0	8.15	107.20	12.99	3.11	1
P-CHLOROANILINE	127.5	72.5	9.08	107.20	12.99	3.11	2
ISOPHTHALONITRILE	128.0	162.0	9.55	118.60	14.24	7.80	2
NAPHTHALENE	128.0	80.55	9.48	123.40	15.56	0.00	4
PHTHALONITRILE	128.0	141.0		118.60	13.24	7.80	2
TEREPHTHALONITRILE	128.0	222.0		118.60	13.24	7.80	4
M-CHLOROPHENOL	128.5	33.0	8.52	103.00	12.29	3.18	1
O-CHLOROPHENOL	128.5	9.0	8.15	103.00	12.29	3.18	1
P-CHLOROPHENOL	128.5	43.5	9.05	103.00	12.29	3.18	2
O-CHLOROFLUOROBENZENE	130.5	-43.0	8.15	99.50	11.66	3.04	2
P-CHLOROFLUOROBENZENE	130.5	-26.8	8.91	99.50	11.66	3.04	2
3-CYANOBENZALDEHYDE	131.0	79.0	9.70	119.30	13.81	6.66	1
4-CYANOBENZALDEHYDE	131.0	101.0	10.17	119.30	13.81	6.66	2
1,2,3,4-TETRAHYDRONAPHTHALENE	132.0	-31.0		137.80	16.08	0.00	1
3-AMINO-2-METHYLBENZONITRILE	132.0	90.0	9.24	129.20	15.10	5.83	1
3-AMINO-4-METHYLBENZONITRILE	132.0	81.0	9.87	129.20	15.10	5.83	1
3-AMINO-5-METHYLBENZONITRILE	132.0	75.0	9.25	129.20	15.10	5.83	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
3-AMINO-6-METHYLBENZONITRILE	132.0	88.0	9.10	129.20	15.10	5.83	1
4-AMINO-2-METHYLBENZONITRILE	132.0	90.0	9.74	129.20	15.10	5.83	1
4-AMINO-3-METHYLBENZONITRILE	132.0	95.0	9.74	129.20	15.10	5.83	1
4-METHYLANTHRANILONITRILE	132.0	94.0	9.74	129.20	15.10	5.83	1
5-METHYLANTHRANILONITRILE	132.0	63.0	9.31	129.20	15.10	5.83	1
6-METHYLANTHRANILONITRILE	132.0	128.0	8.79	129.20	15.10	5.83	1
2-METHOXYBENZONITRILE	133.0	24.5	9.03	123.10	14.45	5.55	1
4-METHOXYBENZONITRILE	133.0	61.0	10.92	123.10	14.45	5.55	2
1,2,3,4-TETRAMETHYLBENZENE	134.0	-6.2	9.08	150.00	16.92	1.60	2
1,2,3,5-TETRAMETHYLBENZENE	134.0	-24.1	9.08	150.00	16.92	1.60	2
1,2,4,5-TETRAMETHYLBENZENE	134.0	79.0	9.08	150.00	16.92	1.60	4
1,2-DIETHYLBENZENE	134.0	-31.0		149.20	16.92	0.80	1
1,4-DIETHYLBENZENE	134.0	-42.8		149.20	16.92	0.80	1
2,4-DIMETHYLBENZALDEHYDE	134.0	-9.0	9.55	135.00	15.15	3.56	1
2-METHYLPROPYLBENZENE	134.0	-51.5		148.80	16.92	0.80	1
2-PHENYL-2-METHYLPROPANE	134.0	-58.1		148.80	16.92	1.20	1
2-PHENYLBUTANE	134.0	-82.7		148.80	16.92	0.80	1
3,5-DIMETHYLBENZALDEHYDE	134.0	9.0	9.29	135.00	15.15	3.56	2
4-METHYLETHYL-1-METHYLBENZENE	134.0	-67.9		149.20	16.92	1.20	1
M-PHTHALALDEHYDE	134.0	90.0	9.73	120.00	13.38	5.52	2
N-BUTYLBENZENE	134.0	-88.5		148.80	16.92	0.40	1
O-PHTHALALDEHYDE	134.0	56.0	8.52	120.00	13.38	5.52	2
P-PHTHALALDEHYDE	134.0	116.0	10.00	120.00	13.38	5.52	4
2,4,5-TRIMETHYLANILINE	135.0	68.0	9.19	144.90	16.44	2.73	1
2,4,6-TRIMETHYLANILINE	135.0	-5.0	9.10	144.90	16.44	2.73	2
2-METHYLBENZAMIDE	135.0	147.0		129.50	14.67	4.02	1
3-METHYLBENZAMIDE	135.0	97.0		129.50	14.67	4.02	1
4-METHYLBENZAMIDE	135.0	160.0		129.50	14.67	4.02	2
1,2-DIMETHYL-3-METHOXYBENZENE	136.0	29.0	9.92	138.80	15.79	2.45	1
2,4-DIMETHYL-1-METHOXYBENZENE	136.0	15.0	10.24	138.80	15.79	2.45	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2-METHOXYBENZALDEHYDE	136.0	37.0	9.15	123.80	14.02	4.41	1
4-METHOXYBENZALDEHYDE	136.0	0.0	10.64	123.80	14.02	4.41	2
M-METHYLBENZOIC ACID	136.0	111.0	10.12	125.30	13.97	2.04	1
O-METHYLBENZOIC ACID	136.0	107.0	9.31	125.30	13.97	2.04	1
P-METHYLBENZOIC ACID	136.0	179.0	10.22	125.30	13.97	2.04	2
2-AMINOBENZAMIDE	136.0	110.0	9.2	124.40	14.19	5.15	1
3-AMINOBENZAMIDE	136.0	113.0	9.96	124.40	14.19	5.15	1
4-AMINOBENZAMIDE	136.0	183.0	10.21	124.40	14.19	5.15	2
2-CHLORO-4-NITROANILINE	136.5	108.0	9.50	105.50	11.42	7.09	1
2-AMINO-3-METHOXYTOLUENE	137.0	31.0	9.92	133.70	15.31	3.58	1
2-AMINO-4-METHOXYTOLUENE	137.0	47.0	10.24	133.70	15.31	3.58	1
2-AMINO-5-METHOXYTOLUENE	137.0	29.0	10.18	133.70	15.31	3.58	1
2-NITROTOLUENE	137.0	-11.0	8.35	120.40	13.70	4.38	1
3,4,5-TRIAMINOTOLUENE	137.0	105.0	9.03	134.70	15.48	4.99	2
3-AMINO-4-METHOXYTOLUENE	137.0	93.0	10.24	133.70	15.31	3.58	1
3-AMINOBENZOIC ACID	137.0	180.0	9.90	120.20	13.49	3.17	1
3-NITROTOLUENE	137.0	15.0	9.17	120.40	13.70	4.38	1
4-AMINO-2-METHOXYTOLUENE	137.0	58.0	9.89	133.70	15.31	3.58	1
4-AMINOBENZOIC ACID	137.0	187.0	10.18	120.20	13.49	3.17	2
4-NITROTOLUENE	137.0	51.0	9.35	120.40	13.70	4.38	2
5-METHOXY-M-TOLUIDINE	137.0	59.0		133.70	15.31	3.58	1
O-AMINOBENZOIC ACID	137.0	146.0	9.31	120.20	13.49	3.17	1
2-HYDROXYBENZAMIDE	137.0	140.0	9.20	120.20	13.49	5.22	1
3-HYDROXYBENZAMIDE	137.0	170.5	9.92	120.20	13.49	5.22	1
4-HYDROXYBENZAMIDE	137.0	162.0	10.15	120.20	13.49	5.22	2
2-CHLOROBENZONITRILE	137.5	43.0	8.89	114.00	13.90	5.48	2
3-CHLOROBENZONITRILE	137.5	40.0	8.94	114.00	13.90	5.48	2
4-CHLOROBENZONITRILE	137.5	94.0	9.94	114.00	13.90	5.48	4
1,2-DIMETHOXYBENZENE	138.0	22.5	9.32	127.60	14.66	3.30	2
1,3-DIMETHOXYBENZENE	138.0	-55.0	11.06	127.60	14.66	3.30	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,4-DIMETHOXYBENZENE	138.0	56.0	11.53	127.60	14.66	3.30	4
1-FLUORO-2,4,6-TRIMETHYLBENZENE	138.0	-36.7	8.96	137.20	15.11	2.66	6
2,4-DIHYDROXYBENZALDEHYDE	138.0	201.0	9.40	116.40	12.79	5.96	1
2,5-DIHYDROXYBENZALDEHYDE	138.0	99.0	9.20	116.40	12.79	5.96	1
2-HYDROXYBENZOIC ACID	138.0	159.0	9.31	116.00	12.79	3.24	1
3,4-DIHYDROXYBENZALDEHYDE	138.0	153.0	9.40	116.40	12.79	5.96	1
4-HYDROXY-3-METHOXYTOLUENE	138.0	5.5	9.92	129.50	14.61	3.65	1
M-HYDROXYBENZOIC ACID	138.0	201.5	9.99	116.00	12.79	3.24	1
M-NITROANILINE	138.0	114.0	9.08	115.30	13.22	5.51	1
O-NITROANILINE	138.0	71.5	8.35	115.30	13.22	5.51	1
P-HYDROXYBENZOIC ACID	138.0	214.5	10.12	116.00	12.79	3.24	2
P-NITROANILINE	138.0	148.0	9.27	115.30	13.22	5.51	2
M-NITROPHENOL	139.0	97.0	9.07	111.10	12.52	5.58	1
O-NITROPHENOL	139.0	44.9	8.35	111.10	12.52	5.58	1
P-NITROPHENOL	139.0	114.0	9.29	111.10	12.52	5.58	2
2-FLUOROBENZOIC ACID	140.0	123.0	9.40	112.50	12.16	3.10	2
3,4,5-TRIHYDROXYTOLUENE	140.0	129.0	8.93	122.10	13.38	5.20	2
3-FLUOROBENZOIC ACID	140.0	124.0	9.40	112.50	12.16	3.10	2
4-FLUOROBENZOIC ACID	140.0	185.0	9.70	112.50	12.16	3.10	2
1,2-DIMETHYL-4-CHLOROBENZENE	140.5	-6.0	9.18	129.70	15.24	2.38	1
1,4-DIMETHYL-2-CHLOROBENZENE	140.5	2.0	9.08	129.70	15.24	2.38	1
2-CHLOROBENZALDEHYDE	140.5	11.0	8.52	114.70	13.47	4.34	1
3-CHLOROBENZALDEHYDE	140.5	18.0	9.09	114.70	13.47	4.34	1
4-CHLOROBENZALDEHYDE	140.5	48.0	9.52	114.70	13.47	4.34	2
1-FLUORO-2-NITROBENZENE	141.0	-6.0	8.35	107.60	11.89	5.44	2
1-FLUORO-3-NITROBENZENE	141.0	41.0	8.65	107.60	11.89	5.44	2
1-FLUORO-4-NITROBENZENE	141.0	27.0	9.15	107.60	11.89	5.44	2
2-AMINO-4-CHLOROTOLUENE	141.5	24.0	9.08	124.60	14.76	3.51	1
2-AMINO-5-CHLOROTOLUENE	141.5	29.0	9.08	124.60	14.76	3.51	1
2-AMINO-6-CHLOROTOLUENE	141.5	1.0	8.50	124.60	14.76	3.51	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
3-AMINO-4-CHLOROTOLUENE	141.5	30.0	9.18	124.60	14.76	3.51	1
4-AMINO-2-CHLOROTOLUENE	141.5	26.0	9.03	124.60	14.76	3.51	1
4-AMINO-3-CHLOROTOLUENE	141.5	7.0	9.03	124.60	14.76	3.51	1
4-CHLORO-M-TOLUIDINE	141.5	83.0		124.60	14.76	3.51	1
1,2,3,5-TETRAHYDROXYBENZENE	142.0	165.0	8.84	112.80	12.20	6.40	2
1,2,4,5-TETRAHYDROXYBENZENE	142.0	215.0	8.84	112.80	12.20	6.40	4
1-METHYLNAPHTHALENE	142.0	-22.0	9.50	140.80	17.33	0.40	1
2-METHYLNAPHTHALENE	142.0	34.6	10.24	140.80	17.33	0.40	1
5-NITRO-M-TOLUONITRILE	142.0	104.5		136.00	15.01	8.20	2
1-CHLORO-2,4-DIAMINOBENZENE	142.5	91.0	9.05	119.50	14.28	4.64	1
1-CHLORO-2,5-DIAMINOBENZENE	142.5	64.0	8.96	119.50	14.28	4.64	1
1-CHLORO-2,6-DIAMINOBENZENE	142.5	85.0	8.85	119.50	14.28	4.64	2
1-CHLORO-3,4-DIAMINOBENZENE	142.5	76.0	9.00	119.50	14.28	4.64	1
1-CHLORO-3,5-DIAMINOBENZENE	142.5	105.0	8.72	119.50	14.28	4.64	2
2-CHLORO-3-HYDROXYTOLUENE	142.5	56.0	8.74	120.40	14.06	3.58	1
2-CHLORO-4-HYDROXYTOLUENE	142.5	56.0	8.93	120.40	14.06	3.58	1
2-CHLORO-5-HYDROXYTOLUENE	142.5	67.0	9.05	120.40	14.06	3.58	1
2-CHLORO-6-HYDROXYTOLUENE	142.5	86.0	8.52	120.40	14.06	3.58	1
2-METHOXY-CHLOROBENZENE	142.5	-27.0	9.32	118.50	14.11	3.23	1
4-CHLORO-2-HYDROXYTOLUENE	142.5	74.0	9.18	120.40	14.06	3.58	1
4-CHLORO-3-HYDROXYTOLUENE	142.5	46.0	9.18	120.40	14.06	3.58	1
4-CHLOROANISOLE	142.5	-18.0	10.34	118.50	14.11	3.23	2
5-CHLORO-2-HYDROXYTOLUENE	142.5	51.0	9.05	120.40	14.06	3.58	1
1-AMINONAPHTHALENE	143.0	50.0	9.48	135.70	16.85	1.53	1
2-AMINONAPHTHALENE	143.0	113.0	10.48	135.70	16.85	1.53	1
1-FLUORONAPHTHALENE	146.0	-9.0	9.54	128.00	15.52	1.46	1
2-FLUORONAPHTHALENE	146.0	61.0	9.85	128.00	15.52	1.46	1
PHTHALIC ACID, MONONITRILE, MONOAMIDE	146.0	175.0		131.20	14.60	7.52	1
1-BROMO-6-HYDROXYNAPHTHALENE	146.9	105.0	10.21	150.70	19.07	3.14	1
2-ETHOXYBENZONITRILE	147.0	5.0	10.44	140.10	16.22	5.55	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
4-CYANOBENZOIC ACID	147.0	219.0		127.00	13.90	5.54	2
4-ETHOXYBENZONITRILE	147.0	61.0	11.91	140.10	16.22	5.55	2
M-DICHLOROBENZENE	147.0	-24.7	8.32	109.40	13.56	3.16	2
O-DICHLOROBENZENE	147.0	-17.0	8.15	109.40	13.56	3.16	2
P-DICHLOROBENZENE	147.0	53.1	9.21	109.40	13.56	3.16	4
(2,2-DIMETHYLPROPYL)BENZENE	148.0	25.0		165.80	18.69	1.20	1
2,4,6-TRIMETHYLBENZALDEHYDE	148.0	14.0	11.10	152.40	16.92	3.96	2
PENTAMETHYLBENZENE	148.0	54.3	9.08	167.40	18.69	2.00	2
2,3,4,5-TETRAMETHYLANILINE	149.0	70.0	9.19	162.30	18.21	3.13	1
2,3,4,6-TETRAMETHYLANILINE	149.0	23.0	9.19	162.30	18.21	3.13	1
1,2,4,5-TETRAFLUOROBENZENE	150.0	4.0	8.61	98.80	9.68	5.84	12
2,3-DIMETHYLBENZOIC ACID	150.0	144.0	10.05	142.70	15.74	2.44	1
2,5-DIMETHYLBENZOIC ACID	150.0	132.0	10.05	142.70	15.74	2.44	1
2,6-DIMETHYLBENZOIC ACID	150.0	116.0	9.18	142.70	15.74	2.44	2
2-FORMYL BENZOIC ACID	150.0	98.0	9.31	127.70	13.97	4.40	1
3,4-DIMETHYLBENZOIC ACID	150.0	166.0	10.24	142.70	15.74	2.44	1
3,5-DIMETHYLBENZOIC ACID	150.0	170.0	10.05	142.70	15.74	2.44	2
3-FORMYL BENZOIC ACID	150.0	175.0	10.55	127.70	13.97	4.40	1
4-FORMYL BENZOIC ACID	150.0	256.0	10.78	127.70	13.97	4.40	2
1,2-DIMETHYL-4-NITROBENZENE	151.0	31.0	9.35	137.80	15.47	4.78	1
1,3-DIMETHYL-2-NITROBENZENE	151.0	13.0	8.96	137.80	15.47	4.78	2
1,3-DIMETHYL-5-NITROBENZENE	151.0	75.0	9.17	137.80	15.47	4.78	2
2,4-DIMETHYL-1-NITROBENZENE	151.0	9.0	9.35	137.80	15.47	4.78	1
2-AMINO-3-METHYLBENZOIC ACID	151.0	172.0		137.60	15.26	3.57	1
2-NITROBENZALDEHYDE	151.0	41.0	8.52	122.80	13.70	6.74	1
3-AMINO BENZOIC AC. METHYL ESTER	151.0	39.0	10.43	135.70	15.26	3.76	1
3-AMINO-4-METHYLBENZOIC ACID	151.0	164.0	10.44	137.60	15.26	3.57	1
3-AMINO-6-METHYLBENZOIC ACID	151.0	198.0	10.10	137.60	15.26	3.57	1
3-NITROBENZALDEHYDE	151.0	58.0	9.15	122.80	13.70	6.74	1
4-AMINO-3-METHYLBENZOIC ACID	151.0	170.0	11.30	137.60	15.26	3.57	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
4-AMINOBENZOIC ACID METHYL ESTER	151.0	114.0	11.15	135.70	15.26	3.76	2
4-NITROBENZALDEHYDE	151.0	106.0	9.85	122.80	13.70	6.74	2
5-METHYLANTHRANILIC ACID	151.0	175.0	10.10	137.60	15.26	3.57	1
2-METHOXYBENZAMIDE	151.0	129.0	9.55	135.70	15.31	5.27	1
4-METHOXYBENZAMIDE	151.0	166.0	15.90	135.70	15.31	5.27	2
2,4-DIAMINOBENZOIC ACID	152.0	140.0	10.15	132.50	14.78	4.70	1
2,6-DIHYDROXY-4-METHYLBENZALDEHYDE	152.0	124.0	9.55	133.80	14.56	6.36	2
2-AMINO-3-NITROTOLUENE	152.0	97.0	9.17	132.70	14.99	5.91	1
2-AMINO-4-NITROTOLUENE	152.0	108.0	9.35	132.70	14.99	5.91	1
2-AMINO-5-NITROTOLUENE	152.0	131.0	9.35	132.70	14.99	5.91	1
2-AMINO-6-NITROTOLUENE	152.0	95.0	9.08	132.70	14.99	5.91	1
2-HYDROXY-3-METHOXYBENZALDEHYDE	152.0	44.0	10.49	131.90	14.61	6.01	1
2-HYDROXY-4-METHOXYBENZALDEHYDE	152.0	40.0	10.75	131.90	14.61	6.01	1
2-HYDROXY-5-METHOXYBENZALDEHYDE	152.0	4.0	10.47	131.90	14.61	6.01	1
2-METHOXY BENZOIC ACID	152.0	101.0	9.31	131.50	14.61	3.29	1
3,4-DIMETHOXYTOLUENE	152.0	22.0	10.24	145.00	16.43	3.70	1
3,5-DIAMINOBENZOIC ACID	152.0	240.0	9.93	132.50	14.78	4.70	2
3-AMINO-2-NITROTOLUENE	152.0	108.0	8.77	132.70	14.99	5.91	1
3-AMINO-4-NITROTOLUENE	152.0	112.0	9.35	132.70	14.99	5.91	1
3-AMINO-5-NITROTOLUENE	152.0	99.0	9.17	132.70	14.99	5.91	1
3-HYDROXY-4-METHOXYBENZALDEHYDE	152.0	116.0	10.65	131.90	14.61	6.01	1
3-HYDROXY-5-METHOXYBENZALDEHYDE	152.0	130.0	10.47	131.90	14.61	6.01	1
3-METHOXYBENZOIC ACID	152.0	110.0	11.17	131.50	14.61	3.29	1
4-AMINO-2-NITROTOLUENE	152.0	79.0	9.03	132.70	14.99	5.91	1
4-AMINO-3-NITROTOLUENE	152.0	117.0	9.17	132.70	14.99	5.91	1
4-HYDROXY-2-METHOXYBENZALDEHYDE	152.0	153.0	9.65	131.90	14.61	6.01	1
4-HYDROXY-3-METHOXYBENZALDEHYDE	152.0	77.0	10.45	131.90	14.61	6.01	1
4-METHOXYBENZOIC ACID	152.0	185.0	11.54	131.50	14.61	3.29	2
5-AMINO-2-NITROTOLUENE	152.0	136.0	9.27	132.70	14.99	5.91	1
2,4-DIMETHOXYANILINE	153.0	33.5	10.03	139.90	15.95	4.83	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,6-DIMETHOXYANILINE	153.0	75.0	9.24	139.90	15.95	4.83	2
2-AMINO-3-HYDROXYBENZOIC ACID	153.0	164.0	10.00	128.30	14.08	4.77	1
2-HYDROXY-3-NITROTOLUENE	153.0	70.0	9.17	128.50	14.29	5.98	1
2-HYDROXY-4-NITROTOLUENE	153.0	118.0	9.35	128.50	14.29	5.98	1
2-HYDROXY-5-NITROTOLUENE	153.0	96.0	9.29	128.50	14.29	5.98	1
2-HYDROXY-6-NITROTOLUENE	153.0	147.0	9.07	128.50	14.29	5.98	1
2-NITROANISOLE	153.0	9.0	9.32	126.60	14.34	5.63	1
3,4-DIMETHOXYANILINE	153.0	87.0	10.03	139.90	15.95	4.83	1
3-AMINO-4-HYDROXYBENZOIC ACID	153.0	210.0	10.24	128.30	14.08	4.77	1
3-HYDROXY-4-NITROTOLUENE	153.0	56.0	9.35	128.50	14.29	5.98	1
3-HYDROXY-5-NITROTOLUENE	153.0	91.0	9.17	128.50	14.29	5.98	1
3-NITROANISOLE	153.0	38.0	10.28	126.60	14.34	5.63	1
4-HYDROXY-2-NITROTOLUENE	153.0	79.0	8.93	128.50	14.29	5.98	1
4-HYDROXY-3-NITROTOLUENE	153.0	37.0	9.17	128.50	14.29	5.98	1
4-NITROANISOLE	153.0	54.0	10.53	126.60	14.34	5.63	2
5-HYDROXY-2-NITROTOLUENE	153.0	129.0	9.29	128.50	14.29	5.98	1
PENTAAMINOBENZENE(DECOMPOSE)	153.0	228.0	8.87	141.90	16.29	7.65	2
2,5-DIHYDROXYBENZOIC ACID	154.0	205.0	9.94	124.10	13.38	4.84	1
3,5-DIHYDROXYBENZOIC ACID	154.0	238.0	9.94	124.10	13.38	4.84	2
ACENAPHTHENE	154.0	96.2	9.48	146.80	18.26	0.00	1
BIPHENYL	154.0	71.0	11.80	150.20	18.84	0.00	2
2-CHLOROBENZAMIDE	155.5	142.4	9.55	126.60	14.76	5.20	1
3-CHLOROBENZAMIDE	155.5	135.0	10.20	126.60	14.76	5.20	1
4-CHLOROBENZAMIDE	155.5	179.0	15.60	126.60	14.76	5.20	2
1,2-DIMETHYLNAPHTHALENE	156.0	-1.6	10.47	158.20	19.10	0.80	1
1,3-DIMETHYLNAPHTHALENE	156.0	-6.0	10.50	158.20	19.10	0.80	1
1,4-DIMETHYLNAPHTHALENE	156.0	7.60	9.49	158.20	19.10	0.80	2
1,5-DIMETHYLNAPHTHALENE	156.0	82.0	10.15	158.20	19.10	0.80	2
1,6-DIMETHYLNAPHTHALENE	156.0	-16.9	10.41	158.20	19.10	0.80	1
1,7-DIMETHYLNAPHTHALENE	156.0	-13.9	10.44	158.20	19.10	0.80	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,8-DIMETHYLNAPHTHALENE	156.0	65.0	9.46	158.20	19.10	0.80	2
1-ETHYLNAPHTHALENE	156.0	-13.8		157.80	19.10	0.40	1
2,3-DIMETHYLNAPHTHALENE	156.0	105.0	10.52	158.20	19.10	0.80	2
2,6-DIMETHYLNAPHTHALENE	156.0	109.0	11.62	158.20	19.10	0.80	2
2-ETHYLNAPHTHALENE	156.0	-7.4		157.80	19.10	0.40	1
2-CHLORO-3-HYDROXYBENZALDEHYDE	156.5	139.5	9.20	122.80	14.06	5.94	1
2-CHLORO-4-HYDROXYBENZALDEHYDE	156.5	147.0	9.46	122.80	14.06	5.94	1
2-CHLORO-5-HYDROXYBENZALDEHYDE	156.5	110.0	9.14	122.80	14.06	5.94	1
3-CHLORO-2-HYDROXYBENZALDEHYDE	156.5	55.0	9.46	122.80	14.06	5.94	1
3-CHLORO-4-HYDROXYBENZALDEHYDE	156.5	139.0	9.46	122.80	14.06	5.94	1
4-CHLORO-2-HYDROXYBENZALDEHYDE	156.5	52.5	9.45	122.80	14.06	5.94	1
4-CHLORO-3-HYDROXYBENZALDEHYDE	156.5	121.0	9.45	122.80	14.06	5.94	1
5-CHLORO-2-HYDROXYBENZALDEHYDE	156.5	99.0	9.13	122.80	14.06	5.94	1
M-CHLOROBENZOIC ACID	156.5	158.0	9.84	122.40	14.06	3.22	1
O-CHLOROBENZOIC ACID	156.5	142.0	9.31	122.40	14.06	3.22	1
P-CHLOROBENZOIC ACID	156.5	243.0	10.41	122.40	14.06	3.22	2
BROMOBENZENE	156.9	-31.0	8.41	99.60	12.76	1.54	2
1-AMINO-2-METHYLNAPHTHALENE	157.0	32.0	10.42	153.10	18.62	1.93	1
1-AMINO-3-METHYLNAPHTHALENE	157.0	51.0	10.42	153.10	18.62	1.93	1
1-AMINO-4-METHYLNAPHTHALENE	157.0	51.0	9.48	153.10	18.62	1.93	1
2-AMINO-1-METHYLNAPHTHALENE	157.0	51.0	10.42	153.10	18.62	1.93	1
2-AMINO-6-METHYLNAPHTHALENE	157.0	129.0	11.46	153.10	18.62	1.93	1
4-CHLORO-2-METHOXYANILINE	157.5	52.0	9.20	130.80	15.40	4.76	1
5-CHLORO-2-METHOXYANILINE	157.5	84.0	9.92	130.80	15.40	4.76	1
M-CHLORONITROBENZENE	157.5	46.0	8.95	117.50	13.79	5.56	1
O-CHLORONITROBENZENE	157.5	34.0	8.35	117.50	13.79	5.56	1
P-CHLORONITROBENZENE	157.5	83.6	9.45	117.50	13.79	5.56	2
1-AMINO-2-HYDROXYNAPHTHALENE	159.0	150.0	10.38	143.80	17.44	3.13	1
1-AMINO-6-HYDROXYNAPHTHALENE	159.0	190.6	10.38	143.80	17.44	3.13	1
1-AMINO-7-HYDROXYNAPHTHALENE	159.0	205.0	10.10	143.80	17.44	3.13	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2-AMINO-3-HYDROXYNAPHTHALENE	159.0	235.0	10.43	143.80	17.44	3.13	2
2-AMINO-6-HYDROXYNAPHTHALENE	159.0	192.0	10.98	143.80	17.44	3.13	2
2-AMINO-7-HYDROXYNAPHTHALENE	159.0	201.0	10.57	143.80	17.44	3.13	2
3,6-DIHYDROXYPHTHAONITRILE	160.0	230.0		134.80	14.42	11.00	2
1-AMINO-4-FLUORONAPHTHALENE	161.0	48.0	9.50	140.30	16.81	2.99	1
2,4-DICHLOROTOLUENE	161.0	-14.0	9.18	126.80	15.33	3.56	1
2,5-DICHLOROTOLUENE	161.0	5.0	9.21	126.80	15.33	3.56	1
3,4-DICHLOROTOLUENE	161.0	-15.0	9.18	126.80	15.33	3.56	1
3,5-DICHLOROTOLUENE	161.0	26.0	8.70	126.80	15.33	3.56	6
2,3-DICHLOROANILINE	162.0	24.0	8.22	121.70	14.85	4.69	1
2,4-DICHLOROANILINE	162.0	63.0	9.12	121.70	14.85	4.69	1
2,5-DICHLOROANILINE	162.0	50.0	9.25	121.70	14.85	4.69	1
2,6-DICHLOROANILINE	162.0	39.0	8.19	121.70	14.85	4.69	2
2-METHYL-5-NITROBENZONITRILE	162.0	106.0	9.41	139.50	15.90	8.28	1
2-NITRO-P-TOLUONITRILE	162.0	101.0		139.50	15.40	8.28	1
3,4-DICHLOROANILINE	162.0	72.0	9.10	121.70	14.85	4.69	1
3,5-DICHLOROANILINE	162.0	51.0	8.19	121.70	14.85	4.69	2
3-NITRO-P-TOLUONITRILE	162.0	107.0		139.50	15.40	8.28	1
4-NITRO-M-TOLUONITRILE	162.0	80.0		139.50	15.40	8.28	1
4-NITRO-O-TOLUONITRILE	162.0	100.0		139.50	15.40	8.28	1
6-NITRO-M-TOLUONITRILE	162.0	93.0		139.50	15.40	8.28	1
6-NITRO-O-TOLUONITRILE	162.0	109.0		139.50	15.40	8.28	1
HEXAMETHYLBENZENE	162.0	165.0	9.08	184.80	20.46	2.40	12
1-CHLORONAPHTHALENE	162.5	-2.3	9.45	137.90	17.42	1.58	1
2-CHLORONAPHTHALENE	162.5	61.0	10.53	137.90	17.42	1.58	1
2,4-DIMETHOXYBENZONITRILE	163.0	96.0	11.00	146.70	16.86	7.20	1
2,5-DIMETHOXYBENZONITRILE	163.0	82.0	11.25	146.70	16.86	7.20	1
2,6-DIMETHOXYBENZONITRILE	163.0	118.0	10.95	146.70	16.86	7.20	2
2-ACETAMIDOBENZALDEHYDE	163.0	70.0	11.63	149.40	16.50	6.36	1
3,4-DIMETHOXYBENZONITRILE	163.0	67.0	11.04	146.70	16.86	7.20	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
3-ACETAMIDOBENZALDEHYDE	163.0	84.0	11.71	149.40	16.50	6.36	1
4-ACETAMIDOBENZALDEHYDE	163.0	156.0	12.02	149.40	16.50	6.36	2
PENTAMETHYLANILINE	163.0	152.0	9.19	179.70	19.98	3.53	2
ISOPHTHALAMIDE	164.0	280.0		143.80	15.96	7.24	2
PHTHALAMIDE	164.0	228.0		143.80	15.96	7.24	2
1,3,5-TRIMETHYL-2-NITROBENZENE	165.0	41.0	9.35	155.20	17.24	5.18	2
1-NITRO-2,3,5-TRIMETHYLBENZENE	165.0	20.0	9.17	155.20	17.24	5.18	1
2,4,5-TRIMETHYLNITROBENZENE	165.0	71.0	9.35	155.20	17.24	5.18	1
3,4,5-TRIMETHYLNITROBENZENE	165.0	20.0	9.35	155.20	17.24	5.18	2
PHTHALIC ACID MONOAMIDE	165.0	148.0		139.60	15.26	5.26	2
TEREPHTHALIC ACID MONOAMIDE	165.0	300.0		139.60	15.26	5.26	4
1,2-DIETHOXYBENZENE	166.0	44.0	11.25	161.60	18.20	3.30	2
1,3-DIETHOXYBENZENE	166.0	12.4	13.10	161.60	18.20	3.30	2
1,4-DIETHOXYBENZENE	166.0	72.0	13.50	161.60	18.20	3.30	4
2,3-DIMETHYL-4-NITROANILINE	166.0	114.0	9.36	150.10	16.76	6.31	1
2,3-DIMETHYL-5-NITROANILINE	166.0	111.0	9.48	150.10	16.76	6.31	1
2,3-DIMETHYL-6-NITROANILINE	166.0	118.0	9.48	150.10	16.76	6.31	1
2,4-DIMETHOXYBENZALDEHYDE	166.0	72.0	10.65	147.40	16.43	6.06	1
2,5-DIMETHOXYBENZALDEHYDE	166.0	52.0	11.25	147.40	16.43	6.06	1
2,6-DIMETHYL-3-NITROANILINE	166.0	81.0	9.35	150.10	16.76	6.31	1
2,6-DIMETHYL-4-NITROANILINE	166.0	76.0	9.33	150.10	16.76	6.31	2
2-ETHOXYBENZOIC ACID	166.0	20.0	10.70	148.50	16.38	3.29	1
3,4-DIMETHOXYBENZALDEHYDE	166.0	44.0	10.62	147.40	16.43	6.06	1
3,4-DIMETHYL-2-NITROANILINE	166.0	65.0	8.90	150.10	16.76	6.31	1
3,4-DIMETHYL-5-NITROANILINE	166.0	74.0	8.90	150.10	16.76	6.31	1
3,5-DIMETHOXYBENZALDEHYDE	166.0	44.5	11.12	147.40	16.43	6.06	2
3,5-DIMETHYL-2-NITROANILINE	166.0	56.0	9.27	150.10	16.76	6.31	1
3,5-DIMETHYL-4-NITROANILINE	166.0	133.0	9.33	150.10	16.76	6.31	2
3-ETHOXYBENZOIC ACID	166.0	137.0	12.24	148.50	16.38	3.29	1
4,5-DIMETHYL-2-NITROANILINE	166.0	140.0	9.31	150.10	16.76	6.31	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
4-ETHOXYBENZOIC ACID	166.0	198.5	12.72	148.50	16.38	3.29	2
FLUORENE	166.0	116.0	11.58	156.60	19.77	0.00	1
M-PHTHALIC ACID	166.0	345.0	11.25	135.40	14.56	3.28	2
O-PHTHALIC ACID	166.0	206.0	9.31	135.40	14.56	3.28	2
P-PHTHALIC ACID(SUBLIMATES)	166.0		11.47	135.40	14.56	3.28	4
2-NITROBENZAMID	166.0	176.6	9.20	134.70	14.99	7.60	1
3-NITROBENZAMID	166.0	142.7	10.36	134.70	14.99	7.60	1
4-NITROBENZAMID	166.0	201.4	10.39	134.70	14.99	7.60	2
2-HYDROXY-3-NITROBENZALDEHYDE	167.0	109.0	9.68	130.90	14.29	8.34	1
2-HYDROXY-5-NITROBENZALDEHYDE	167.0	128.0	9.17	130.90	14.29	8.34	1
3-AMINO-4-HYDROXYBENZOIC AC.METHYL ESTER	167.0	143.0	10.45	143.80	15.85	5.36	1
3-HYDROXY-2-NITROBENZALDEHYDE	167.0	152.0	8.45	130.90	14.29	8.34	1
3-HYDROXY-4-NITROBENZALDEHYDE	167.0	128.0	9.86	130.90	14.29	8.34	1
4-AMINO-2-HYDROXYBENZOIC ACID METHYL EST	167.0	120.0	11.15	143.80	15.85	5.36	1
4-HYDROXY-2-NITROBENZALDEHYDE	167.0	67.0	9.43	130.90	14.29	8.34	1
4-HYDROXY-3-NITROBENZALDEHYDE	167.0	144.3	9.59	130.90	14.29	8.34	1
M-NITROBENZOIC ACID	167.0	141.0	10.38	130.50	14.29	5.62	1
O-NITROBENZOIC ACID	167.0	147.0	9.31	130.50	14.29	5.62	1
P-NITROBENZOIC ACID	167.0	242.0	10.57	130.50	14.29	5.62	2
1,1-DIPHENYLETHYLENE	168.0	8.2		172.20	21.19	0.40	2
1,2,3-TRIMETHOXYBENZENE	168.0	47.0	11.06	151.20	17.07	4.95	2
1,3,5-TRIMETHOXYBENZENE	168.0	54.0	11.06	151.20	17.07	4.95	6
2-METHOXY-3-NITROANILINE	168.0	67.0	9.20	138.90	15.63	7.16	1
2-METHYLBIPHENYL	168.0	-0.2	11.80	167.60	20.61	0.40	1
2-NITRO-5-METHOXYANILINE	168.0	131.0	10.55	138.90	15.63	7.16	1
3-AMINO-2-HYDROXY-5-NITROTOLUENE	168.0	176.0	9.29	140.80	15.58	7.51	1
3-AMINO-4-HYDROXY-5-NITROTOLUENE	168.0	119.0	9.17	140.80	15.58	7.51	1
3-METHYLBIPHENYL	168.0	4.5	11.91	167.60	20.61	0.40	1
4-METHYLBIPHENYL	168.0	49.0	12.64	167.60	20.61	0.40	1
5-AMINO-2-HYDROXY-3-NITROTOLUENE	168.0	118.0	9.17	140.80	15.58	7.51	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
5-AMINO-4-HYDROXY-2-NITROTOLUENE	168.0	200.0	9.27	140.80	15.58	7.51	1
DIPHENYLMETHANE	168.0	25.35	12.05	167.20	20.61	0.00	1
M-DINITROBENZENE	168.0	90.2	9.45	125.60	14.02	7.96	2
O-DINITROBENZENE	168.0	118.5	8.35	125.60	14.02	7.96	2
P-DINTROBENZENE	168.0	174.0	9.70	125.60	14.02	7.96	4
2-AMINOBIPHENYL	169.0	51.0	11.80	162.50	20.13	1.53	1
3-AMINOACENAPHTHENE	169.0	81.5	10.15	159.10	19.55	1.53	1
3-AMINOBIPHENYL	169.0	30.0	11.86	162.50	20.13	1.53	1
4-AMINOACENAPHTHENE	169.0	87.0	10.40	159.10	19.55	1.53	1
4-AMINOBIPHENYL	169.0	53.0	12.52	162.50	20.13	1.53	1
5-AMINOACENAPHTHENE	169.0	108.0	9.48	159.10	19.55	1.53	1
1,2,3-TRIMETHYLNAPHTHALENE	170.0	27.0	10.50	175.60	20.87	1.20	1
1,2,4-TRIMETHYLNAPHTHALENE	170.0	55.0	10.41	175.60	20.87	1.20	1
1,2,5-TRIMETHYLNAPHTHALENE	170.0	33.5	10.48	175.60	20.87	1.20	1
1,2,6-TRIMETHYLNAPHTHALENE	170.0	14.0	11.45	175.60	20.87	1.20	1
1,4,5-TRIMETHYLNAPHTHALENE	170.0	58.0	10.30	175.60	20.87	1.20	1
2,3,6-TRIMETHYLNAPHTHALENE	170.0	100.0	11.53	175.60	20.87	1.20	1
2-CHLORO-4-METHYLBENZOIC ACID	170.5	155.0	10.24	139.80	15.83	3.62	1
2-CHLORO-5-METHYLBENZOIC ACID	170.5	167.0	9.94	139.80	15.83	3.62	1
2-CHLORO-6-METHYLBENZOIC ACID	170.5	102.0	9.12	139.80	15.83	3.62	2
3-CHLORO-2-METHYLBENZOIC ACID	170.5	159.0	9.82	139.80	15.83	3.62	1
3-CHLORO-4-METHYLBENZOIC ACID	170.5	200.0	10.24	139.80	15.83	3.62	1
3-CHLORO-5-METHYLBENZOIC ACID	170.5	178.0	9.98	139.80	15.83	3.62	2
4-CHLORO-2-METHYLBENZOIC ACID	170.5	173.0	10.25	139.80	15.83	3.62	1
4-CHLORO-3-METHYLBENZOIC ACID	170.5	209.0	10.25	139.80	15.83	3.62	1
5-CHLORO-2-METHYLBENZOIC ACID	170.5	168.0	9.83	139.80	15.83	3.62	1
M-METHYLBROMOBENZENE	170.9	-40.0	8.93	117.00	14.53	1.94	2
O-METHYLBROMOBENZENE	170.9	-28.0	8.41	117.00	14.53	1.94	2
P-METHYLBROMOBENZENE	170.9	28.5	9.42	117.00	14.53	1.94	4
2-CHLORO-4-NITROTOLUENE	171.5	68.0	9.35	134.90	15.56	5.96	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2-CHLORO-5-NITROTOLUENE	171.5	61.0	9.45	134.90	15.56	5.96	1
2-CHLORO-6-NITROTOLUENE	171.5	39.0	8.95	134.90	15.56	5.96	1
3-CHLORO-4-NITROTOLUENE	171.5	24.0	9.35	134.90	15.56	5.96	1
4-AMINO-2-CHLOROBENZOIC ACID(DEC)	171.5	213.0	10.02	134.70	15.35	4.75	1
4-CHLORO-2-NITROTOLUENE	171.5	38.0	9.18	134.90	15.56	5.96	1
4-CHLORO-3-NITROTOLUENE	171.5	7.0	9.18	134.90	15.56	5.96	1
5-CHLORO-2-ETHOXYANILINE	171.5	42.0	11.27	147.80	17.17	4.76	1
5-CHLORO-2-NITROTOLUENE	171.5	25.0	9.45	134.90	15.56	5.96	1
M-BROMOANILINE	171.9	18.5	8.83	111.90	14.05	3.07	1
O-BROMOANILINE	171.9	32.0	8.41	111.90	14.05	3.07	1
P-BROMOANILINE	171.9	66.4	9.35	111.90	14.05	3.07	2
2-FLUOROBIPHENYL	172.0	73.5	11.54	154.80	18.80	1.46	1
4-FLUOROBIPHENYL	172.0	74.5	11.90	154.80	18.80	1.46	1
3-CHLORO-4-NITROANILINE	172.5	156.0	9.38	129.80	15.08	7.09	1
4-CHLORO-2-NITROANILINE	172.5	116.0	9.20	129.80	15.08	7.09	1
4-CHLORO-3-NITROANILINE	172.5	103.0	9.20	129.80	15.08	7.09	1
5-CHLORO-2-NITROANILINE	172.5	126.5	9.43	129.80	15.08	7.09	1
5-CHLORO-3-NITROANILINE	172.5	133.0	8.24	129.80	15.08	7.09	1
6-CHLORO-2-NITROANILINE	172.5	76.0	8.20	129.80	15.08	7.09	1
6-CHLORO-3-NITROANILINE	172.5	121.0	9.35	129.80	15.08	7.09	1
M-BROMOPHENOL	172.9	33.0	8.81	107.70	13.35	3.14	1
O-BROMOPHENOL	172.9	5.6	8.41	107.70	13.35	3.14	1
P-BROMOPHENOL	172.9	66.4	9.20	107.70	13.35	3.14	2
1-NITRONAPHTHALENE	173.0	61.5	9.54	146.00	17.65	3.98	1
2-NITRONAPHTHALENE	173.0	79.0	10.52	146.00	17.65	3.98	1
HEXAHYDROXYBENZENE	174.0	300.0	8.84	129.00	13.38	9.60	12
4-FLUOROBROMOBENZENE	174.9	-17.0	9.19	104.20	12.72	3.00	2
2,3-DICHLOROBENZALDEHYDE	175.0	65.0	8.50	129.20	15.33	5.92	1
2,4-DICHLOROBENZALDEHYDE	175.0	72.0	9.55	129.20	15.33	5.92	1
2,5-DICHLORO-P-XYLENE	175.0	70.0	9.21	144.20	17.10	3.96	4

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,5-DICHLOROBENZALDEHYDE	175.0	58.0	9.13	129.20	15.33	5.92	1
2,6-DICHLOROBENZALDEHYDE	175.0	71.0	8.50	129.20	15.33	5.92	2
3,4-DICHLORO-O-XYLENE	175.0	76.0	9.18	144.20	17.10	3.96	2
3,4-DICHLOROBENZALDEHYDE	175.0	44.0	9.55	129.20	15.33	5.92	1
3,5-DICHLOROBENZALDEHYDE	175.0	65.0	9.14	129.20	15.33	5.92	2
2,4-DICHLORO-1-METHOXYBENZENE	177.0	29.0	10.14	133.00	15.97	4.81	1
2,4-DICHLORO-3-HYDROXYTOLUENE	177.0	59.0	9.18	134.90	15.92	5.16	1
2,4-DICHLORO-5-HYDROXYTOLUENE	177.0	73.0	9.18	134.90	15.92	5.16	1
2,6-DICHLORO-3-HYDROXYTOLUENE	177.0	27.0	9.05	134.90	15.92	5.16	1
3,5-DICHLORO-2-HYDROXYTOLUENE	177.0	55.0	9.05	134.90	15.92	5.16	2
3,5-DICHLORO-4-HYDROXYTOLUENE	177.0	39.0	8.93	134.90	15.92	5.16	2
4,5-DICHLORO-2-HYDROXYTOLUENE	177.0	101.0	9.18	134.90	15.92	5.16	1
1-AMINO-2-CHLORONAPHTHALENE	177.5	60.0	10.56	150.20	18.71	3.11	1
1-AMINO-4-CHLORONAPHTHALENE	177.5	99.0	9.53	150.20	18.71	3.11	1
2-AMINO-1-CHLORONAPHTHALENE	177.5	60.0	10.13	150.20	18.71	3.11	1
ANTHRACENE	178.0	216.0	12.00	166.40	21.28	0.00	4
PHENANTHRENE	178.0	101.0	11.66	166.40	21.28	0.00	2
2-NITROACETANILIDE	180.0	93.0	10.37	152.20	16.82	7.58	1
3-NITROACETANILIDE	180.0	154.0	11.51	152.20	16.82	7.58	1
4-NITROACETANILIDE	180.0	216.0	11.48	152.20	16.82	7.58	2
5-METHYLISOPHTHALIC ACID	180.0	298.0		152.80	16.33	3.68	2
2,5-DIMETHOXYBENZAMIDE	181.0	141.0	11.08	159.30	17.72	6.92	1
2-AMINOFLUORENE	181.0	131.0	12.40	168.90	21.06	1.53	1
2-METHOXY-3-NITROBENZALDEHYDE	181.0	89.0	9.12	146.40	16.11	8.39	1
3-AMINOPHTHALIC ACID	181.0	231.0	10.05	147.70	15.85	4.81	1
4-AMINO-ISOPHTHALIC ACID	181.0	336.0		147.70	15.85	4.81	1
3,4-DIMETHOXYBENZAMIDE	181.0	164.0	15.90	159.30	17.72	6.92	1
3,5-DIMETHOXYBENZAMIDE	181.0	148.0	11.08	159.30	17.72	6.92	2
1,2,3-TRICHLOROBENZENE	181.5	53.0	8.32	123.90	15.42	4.74	2
1,2,4-TRICHLOROBENZENE	181.5	17.0	9.21	123.90	15.42	4.74	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,3,5-TRICHLOROBENZENE	181.5	63.0	8.32	123.90	15.42	4.74	6
2-BROMOBENZONITRILE	181.9	55.5	8.89	118.70	14.96	5.44	2
3-BROMOBENZONITRILE	181.9	39.0	9.16	118.70	14.96	5.44	2
4-BROMOBENZONITRILE	181.9	114.0	10.20	118.70	14.96	5.44	4
2,2'-DIMETHYLBIPHENYL	182.0	19.0	11.67	185.00	22.38	0.80	1
2,3-DIMETHYLBIPHENYL	182.0	42.0	11.89	185.00	22.38	0.80	1
2,3-DINITROTOLUENE	182.0	61.0	9.17	143.00	15.79	8.36	1
2,4-DIMETHOXY-6-HYDROXYBENZALDEHYDE	182.0	71.0	10.80	155.50	17.02	7.66	1
2,4-DINITROTOLUENE	182.0	71.0	9.35	143.00	15.79	8.36	1
2,5-DINITROTOLUENE	182.0	53.0	9.70	143.00	15.79	8.36	1
2,6-DIMETHOXY-4-HYDROXYBENZALDEHYDE	182.0	70.0	11.24	143.10	17.02	7.66	2
2,6-DIMETHYLBIPHENYL	182.0	-5.0	11.67	185.00	22.38	0.80	1
2,6-DINITROTOLUENE	182.0	66.0	9.45	143.00	15.79	8.36	2
2-HYDROXYFLUORENE	182.0	171.0	12.43	164.70	20.36	1.60	1
2-HYDROXYISOPHTHALIC ACID	182.0	244.0		143.50	15.15	4.88	2
3,3'-DIMETHYLBIPHENYL	182.0	9.0	11.67	185.00	22.38	0.80	1
3,4'-DIMETHYLBIPHENYL	182.0	14.0	12.12	185.00	22.38	0.80	1
3,4-DIMETHOXY-5-HYDROXYBENZALDEHYDE	182.0	62.0	10.62	155.50	17.02	7.66	1
3,4-DIMETHYLBIPHENYL	182.0	29.2	12.12	185.00	22.38	0.80	1
3,4-DINITROTOLUENE	182.0	58.0	9.35	143.00	15.79	8.36	1
3,5-DIMETHOXY-4-HYDROXYBENZALDEHYDE	182.0	113.0	11.12	155.50	17.02	7.66	2
3,5-DIMETHYLBIPHENYL	182.0	22.0	13.00	185.00	22.38	0.80	1
3,5-DINITROTOLUENE	182.0	93.0	9.45	143.00	15.79	8.36	2
3-AMINO-2-NITROBENZOIC ACID	182.0	156.0	10.10	142.80	15.58	7.15	1
3-AMINO-4-NITROBENZOIC ACID(DEC)	182.0	298.0	10.76	142.80	15.58	7.15	1
3-AMINO-5-NITROBENZOIC ACID	182.0	209.0	10.44	142.80	15.58	7.15	1
3-AMINO-6-NITROBENZOIC ACID(DEC)	182.0	253.0	10.10	142.80	15.58	7.15	1
3-NITROANTHRANILIC ACID	182.0	208.0	10.28	142.80	15.58	7.15	1
4,4'-DIMETHYLBIPHENYL	182.0	125.0	11.90	185.00	22.38	0.80	2
4-HYDROXY ISOPHTHALIC ACID	182.0	310.0		143.50	15.15	4.88	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
4-NITROANTHRANILIC ACID	182.0	269.0	10.48	142.80	15.58	7.15	1
5-HYDROXYISOPHTHALIC ACID	182.0			143.50	15.15	4.88	2
6-NITROANTHRANILIC ACID	182.0	184.0	9.20	142.80	15.58	7.15	1
PENTAMETHYLCHLOROBENZENE	182.5	154.0	9.18	181.90	20.55	3.58	12
1,2-DIMETHOXY-3-NITROBENZENE	183.0	98.0	10.20	150.20	16.75	7.28	1
1,3-DIMETHOXY-2-NITROBENZENE	183.0	131.0	10.79	150.20	16.75	7.28	2
1,3-DIMETHOXY-5-NITROBENZENE	183.0	89.0	9.84	150.20	16.75	7.28	2
1,4-DIMETHOXY-2-NITROBENZENE	183.0	72.0	11.53	150.20	16.75	7.28	1
2,3-DINITROANILINE	183.0	178.0	9.27	137.90	15.31	9.49	1
2,4-DIMETHOXY-1-NITROBENZENE	183.0	77.0	10.53	150.20	16.75	7.28	1
2,4-DINITROANILINE	183.0	180.0	8.29	137.90	15.31	9.49	1
2,6-DINITROANILINE	183.0	141.0	9.36	137.90	15.31	9.49	2
3,5-DINITROANILINE	183.0	163.0	8.40	137.90	15.31	9.49	2
PENTAFLUOROANILINE	183.0	34.0	8.31	115.70	10.93	8.83	2
1,2,5,6-TETRAMETHYLNAPHTHALENE	184.0	118.0	11.51	193.00	22.64	1.60	2
1,3,6,8-TETRAMETHYLNAPHTHALENE	184.0	207.0	11.26	193.00	22.64	1.60	2
2,2'-DIAMINOBIPHENYL	184.0	81.0	11.67	174.80	21.42	3.06	1
2,4'-DIAMINOBIPHENYL	184.0	54.0	14.89	174.80	21.42	3.06	1
2-METHOXYBIPHENYL	184.0	29.0	11.80	173.80	21.25	1.65	1
3,3'-DIAMINOBIPHENYL	184.0	93.0	11.67	174.80	21.42	3.06	1
3,4-DIAMINOBIPHENYL	184.0	103.0	12.51	174.80	21.42	3.06	1
4,4'-DIAMINOBIPHENYL	184.0	125.0	13.40	174.80	21.42	3.06	2
4-METHYOXYBIPHENYL	184.0	90.0	13.60	173.80	21.25	1.65	1
1,2-DIMETHYL-4-BROMOBENZENE	184.9	0.0	9.42	134.40	16.30	2.34	1
1,4-DIMETHYL-2-BROMOBENZENE	184.9	9.0	9.08	134.40	16.30	2.34	1
2,4-DIMETHYLBROMOBENZENE	184.9	0.0	9.42	134.40	16.30	2.34	1
2-BROMO-M-XYLENE	184.9	-10.0	8.96	134.40	16.30	2.34	2
2-BROMOBENZALDEHYDE	184.9	21.0	8.52	119.40	14.53	4.30	1
3-BROMOBENZALDEHYDE	184.9	n.a.	9.30	119.40	14.53	4.30	1
4-BROMOBENZALDEHYDE	184.9	67.0	9.85	119.40	14.53	4.30	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA	
5-BROMO-2-HYDROXYTOLUENE	186.9	64.0	9.20	125.10	15.12	3.54	1	
1-METHYL-2-NITRONAPHTHALENE	187.0	58.0	10.81	163.40	19.42	4.38	1	
1-METHYL-3-NITRONAPHTHALENE	187.0	81.0	10.50	163.40	19.42	4.38	1	
1-METHYL-4-NITRONAPHTHALENE	187.0	71.0	9.45	163.40	19.42	4.38	1	
1-METHYL-5-NITRONAPHTHALENE	187.0	82.0	10.54	163.40	19.42	4.38	1	
1-METHYL-6-NITRONAPHTHALENE	187.0	76.0	10.75	163.40	19.42	4.38	1	
1-METHYL-7-NITRONAPHTHALENE	187.0	98.0	10.77	163.40	19.42	4.38	1	
1-METHYL-8-NITRONAPHTHALENE	187.0	65.0	9.43	163.40	19.42	4.38	1	
2-METHYL-1-NITRONAPHTHALENE	187.0	81.0	10.55	163.40	19.42	4.38	1	
2-METHYL-3-NITRONAPHTHALENE	187.0	117.0	10.74	163.40	19.42	4.38	1	
2-METHYL-4-NITRONAPHTHALENE	187.0	49.0	10.44	163.40	19.42	4.38	1	
2-METHYL-5-NITRONAPHTHALENE	187.0	61.0	10.88	163.40	19.42	4.38	1	
2-METHYL-6-NITRONAPHTHALENE	187.0	119.0	11.76	163.40	19.42	4.38	1	
2-METHYL-7-NITRONAPHTHALENE	187.0	105.0	10.87	163.40	19.42	4.38	1	
2-METHYL-8-NITRONAPHTHALENE	187.0	36.0	10.48	163.40	19.42	4.38	1	
2-NITRO-4-CHLOROANISOLE	187.5	98.0	10.14	141.10	16.20	7.21	1	
3-CHLORO-2-NITROANISOLE	187.5	56.0	9.65	141.10	16.20	7.21	1	
1-AMINO-2-NITRONAPHTHALENE	188.0	144.0	10.50	158.30	18.94	5.51	1	
1-AMINO-3-NITRONAPHTHALENE	188.0	137.0	10.77	158.30	18.94	5.51	1	
1-AMINO-4-NITRONAPHTHALENE	188.0	195.0	9.48	158.30	18.94	5.51	1	
1-AMINO-5-NITRONAPHTHALENE	188.0	118.0	10.48	158.30	18.94	5.51	1	
1-AMINO-6-NITRONAPHTHALENE	188.0	172.0	10.83	158.30	18.94	5.51	1	
1-AMINO-8-NITRONAPHTHALENE	188.0	96.0	9.50	158.30	18.94	5.51	1	
2-AMINO-1-NITRONAPHTHALENE	188.0	126.0	10.24	158.30	18.94	5.51	1	
2-AMINO-6-NITRONAPHTHALENE	188.0	207.5	10.78	158.30	18.94	5.51	1	
6-AMINO-1-NITRONAPHTHALENE	188.0	143.5	10.46	158.30	18.94	5.51	1	
7-AMINO-1-NITRONAPHTHALENE	188.0	104.5	10.77	158.30	18.94	5.51	1	
2-CHLOROBIPHENYL	188.5	34.0	11.67	164.70	20.70	1.58	1	
3-CHLOROBIPHENYL	188.5	16.0	11.67	164.70	20.70	1.58	1	
4-CHLOROBIPHENYL	188.5	77.7	12.69	164.70	20.70	1.58	1	

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
5-CHLOROACENAPHTHENE	188.5	70.5	9.90	161.30	20.12	1.58	1
2,4-DICHLOROMESITYLENE	189.0	59.0	9.18	161.60	18.87	4.36	2
2,2'-DIFLUOROBIPHENYL	190.0	118.5	11.80	159.40	18.76	2.92	1
3,3'-DIFLUOROBIPHENYL	190.0	8.0	11.54	159.40	18.76	2.92	1
4,4'-DIFLUOROBIPHENYL	190.0	94.0	12.27	159.40	18.76	2.92	2
4,5-METHYLENEPHENANTHRENE	190.0	116.0	11.69	172.80	22.21	0.00	2
2,3-DICHLOROBENZOIC ACID	191.0	168.0	9.82	136.90	15.92	4.80	1
2,4-DICHLORO-3-HYDROXYBENZALDEHYDE	191.0	141.0	9.55	137.30	15.92	7.52	1
2,4-DICHLOROBENZOIC ACID	191.0	164.2	10.25	136.90	15.92	4.80	1
2,5-DICHLOROBENZOIC ACID	191.0	154.4	9.82	136.90	15.92	4.80	1
2,6-DICHLORO-3-HYDROXYBENZALDEHYDE	191.0	142.0	9.26	137.30	15.92	7.52	1
2,6-DICHLOROBENZOIC ACID	191.0	144.0	9.12	136.90	15.92	4.80	2
3,4-DICHLOROBENZOIC ACID	191.0	208.0	10.25	136.90	15.92	4.80	1
3,5-DICHLORO-2-HYDROXYBENZALDEHYDE	191.0	95.0	9.14	137.30	15.92	7.52	1
3,5-DICHLORO-4-HYDROXYBENZALDEHYDE	191.0	158.0	9.43	137.30	15.92	7.52	2
3,5-DICHLOROBENZOIC ACID	191.0	188.0	9.82	136.90	15.92	4.80	2
4,6-DICHLORO-3-HYDROXYBENZALDEHYDE	191.0	130.0	9.55	137.30	15.92	7.52	1
2-CHLOROBROMOBENZENE	191.4	-12.0	8.41	114.10	14.62	3.12	2
3-CHLOROBROMOBENZENE	191.4	-22.0	8.59	114.10	14.62	3.12	2
4-CHLOROBROMOBENZENE	191.4	68.0	9.49	114.10	14.62	3.12	4
1,2-DICHLORO-3-NITROBENZENE	192.0	62.0	8.95	132.00	15.65	7.14	1
1,2-DICHLORO-4-NITROBENZENE	192.0	43.0	9.45	132.00	15.65	7.14	1
1,3-DICHLORO-2-NITROBENZENE	192.0	73.0	8.35	132.00	15.65	7.14	2
1,3-DICHLORO-5-NITROBENZENE	192.0	65.0	8.95	132.00	15.65	7.14	2
1,4-DICHLORO-2-NITROBENZENE	192.0	56.0	9.21	132.00	15.65	7.14	1
1-METHYLANTHRACENE	192.0	85.0	11.93	183.80	23.05	0.40	1
1-METHYLPHENANTHRENE	192.0	123.0	11.93	183.80	23.05	0.40	1
2,4-DICHLORO-1-NITROBENZENE	192.0	34.0	9.45	132.00	15.65	7.14	1
2-METHYLANTHRACENE	192.0	209.0	13.00	183.80	23.05	0.40	1
4-METHYLPHENANTHRENE	192.0	52.5	11.66	183.80	23.05	0.40	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDH	SIGMA
9-METHYLANTHRACENE	192.0	81.5	11.93	183.80	23.05	0.40	2
9-METHYLPHENANTHRENE	192.0	90.0	11.66	183.80	23.05	0.40	1
PENTAMETHYLBENZOIC ACID	192.0	210.5	10.24	194.90	21.05	3.64	2
1-AMINOANTHRACENE	193.0	130.0	12.00	178.70	22.57	1.53	1
2-AMINOANTHRACENE	193.0	238.0	12.98	178.70	22.57	1.53	1
9-AMINOANTHRACENE	193.0	145.0	11.98	178.70	22.57	1.53	2
1-HYDROXYANTHRACENE	194.0	158.0	11.96	174.50	21.87	1.60	1
2-HYDROXYANTHRACENE	194.0	253.0	12.50	174.50	21.87	1.60	1
4,6-DIMETHYLISOPHTHALIC ACID	194.0	266.0		170.20	18.10	4.08	2
9-HYDROXYANTHRACENE	194.0	160.0	11.94	174.50	21.87	1.60	2
ISOPHTHALIC ACID DIMETHYL ESTER	194.0	67.0		166.40	18.10	4.46	2
TEREPHTHALIC ACID DIMETHYL ESTER	194.0	141.0		166.40	18.10	4.46	4
2,3,4-TRICHLOROTOLUENE	195.5	44.0	9.18	141.30	17.19	5.14	2
2,3,5-TRICHLOROTOLUENE	195.5	46.0	9.21	141.30	17.19	5.14	2
2,3,6-TRICHLOROTOLUENE	195.5	46.0	9.21	141.30	17.19	5.14	2
2,4,5-TRICHLOROTOLUENE	195.5	85.0	9.21	141.30	17.19	5.14	4
2,4,6-TRICHLOROTOLUENE	195.5	38.0	9.18	141.30	17.19	5.14	2
3,4,5-TRICHLOROTOLUENE	195.5	45.0	9.18	141.30	17.19	5.14	2
3-CHLORO-2,6-DINITROANILINE	195.5	112.0	9.50	146.80	15.57	11.07	1
1,2-DIMETHYL-3,4-DINITROBENZENE	196.0	82.0	9.35	160.40	17.56	8.76	1
1,2-DIMETHYL-3,5-DINITROBENZENE	196.0	77.0	9.45	160.40	17.56	8.76	1
1,2-DIMETHYL-4,5-DINITROBENZENE	196.0	118.0	9.35	160.40	17.56	8.76	2
1,3-DIMETHYL-2,5-DINITROBENZENE	196.0	101.0	9.70	160.40	17.56	8.76	2
1,4-DIMETHYL-2,3-DINITROBENZENE	196.0	93.0	9.17	160.40	17.56	8.76	2
1,4-DIMETHYL-2,5-DINITROBENZENE	196.0	147.0	9.70	160.40	17.56	8.76	2
2,3-DIMETHYL-1,4-DINITROBENZENE	196.0	90.0	9.70	160.40	17.56	8.76	2
2,4,5-TRIMETHOXYBENZALDEHYDE	196.0	114.0	11.07	171.00	18.84	7.71	1
2,4-DINITROBENZALDEHYDE	196.0	72.0	9.82	145.40	15.79	10.72	1
2,5-DIMETHYL-1,3-DINITROBENZENE	196.0	123.0	9.45	160.40	17.56	8.76	2
2,6-DINITROBENZALDEHYDE	196.0	123.0	9.57	145.40	15.79	10.72	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,7-DIAMINOFLUORENE	196.0	165.0	13.30	181.20	22.35	3.06	1
3,4,5-TRIMETHOXYBENZALDEHYDE	196.0	90.0	11.10	171.00	18.84	7.71	2
2,3,4-TRICHLOROANILINE	196.5	73.0	9.00	136.20	16.71	6.27	1
2,4,5-TRICHLOROANILINE	196.5	96.5	9.29	136.20	16.71	6.27	1
2,4,6-TRICHLOROANILINE	196.5	78.5	8.22	136.20	16.71	6.27	2
1,2-DICHLORONAPHTHALENE	197.0	35.0	10.53	152.40	19.28	3.16	1
1,3-DICHLORONAPHTHALENE	197.0	61.5	10.48	152.40	19.28	3.16	1
1,4-DICHLORONAPHTHALENE	197.0	68.0	9.48	152.40	19.28	3.16	2
1,5-DICHLORONAPHTHALENE	197.0	107.0	9.74	152.40	19.28	3.16	2
1,6-DICHLORONAPHTHALENE	197.0	49.0	10.52	152.40	19.28	3.16	1
1,7-DICHLORONAPHTHALENE	197.0	63.0	10.51	152.40	19.28	3.16	1
1,8-DICHLORONAPHTHALENE	197.0	89.0	9.48	152.40	19.28	3.16	2
2,3-DICHLORONAPHTHALENE	197.0	120.0	10.54	152.40	19.28	3.16	2
2,6-DICHLORONAPHTHALENE	197.0	140.0	11.58	152.40	19.28	3.16	2
2,7-DICHLORONAPHTHALENE	197.0	114.0	10.88	152.40	19.28	3.16	2
4-AMINO-2,6-DINITROTOLUENE	197.0	171.0	9.45	155.30	17.08	9.89	2
1,2-DINITRO-3-METHOXYBENZENE	198.0	119.0	10.28	149.20	16.43	9.61	1
1,2-DINITRO-4-METHOXYBENZENE	198.0	71.0	10.53	149.20	16.43	9.61	1
1,3-DINITRO-2-METHOXYBENZENE	198.0	118.0	9.70	149.20	16.43	9.61	2
1,3-DINITRO-5-METHOXYBENZENE	198.0	105.0	10.28	149.20	16.43	9.61	2
1,4-DINITRO-2-METHOXYBENZENE	198.0	97.0	10.28	149.20	16.43	9.61	1
2,4-DINITRO-1-METHOXYBENZENE	198.0	95.0	10.53	149.20	16.43	9.61	1
2,4-DINITRO-6-HYDROXYTOLUENE	198.0	86.0	9.45	151.10	16.38	9.96	1
2-CARBOXYLIC ACID BIPHENYL	198.0	113.0	11.80	177.70	21.20	1.64	1
2-ETHOXYBIPHENYL	198.0	34.0	11.80	190.80	23.02	1.65	1
3,5-DINITRO-2-HYDROXYTOLUENE	198.0	85.0	9.45	151.10	16.38	9.96	1
3-CARBOXYLIC ACID BIPHENYL	198.0	165.0	13.15	177.70	21.20	1.64	1
3-ETHOXYBIPHENYL	198.0	35.0	13.99	190.80	23.02	1.65	1
4-CARBOXYLIC ACID BIPHENYL	198.0	228.0	13.72	177.70	21.20	1.64	1
5-CARBOXYLIC ACID ACENAPHTHENE	198.0	220.0	11.38	174.30	20.62	1.64	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,3,5-TRIMETHYL-2-BROMOBENZENE	198.9	-1.0	9.42	151.80	18.07	2.74	2
2,4,5-TRIMETHYLBROMOBENZENE	198.9	73.0	9.42	151.80	18.07	2.74	4
2,4,4'-TRIAMINOBIPHENYL	199.0	134.0	13.55	187.10	22.71	4.59	1
2-NITROBIPHENYL	199.0	37.2	11.80	172.80	20.93	3.98	1
3-NITROACENAPHTHENE	199.0	151.5	10.80	169.40	20.35	3.98	1
3-NITROBIPHENYL	199.0	62.0	12.22	172.80	20.93	3.98	1
4-NITROBIPHENYL	199.0	114.0	12.85	172.80	20.93	3.98	1
5-NITROACENAPHTHENE	199.0	103.4	10.46	169.40	20.35	3.98	1
2-BROMOBENZAMIDE	199.9	160.0	9.55	131.30	15.82	5.16	1
3-BROMOBENZAMIDE	199.9	155.3	10.30	131.30	15.82	5.16	1
4-BROMOBENZAMIDE	199.9	192.0	10.84	131.30	15.82	5.16	2
2-CHLOROTEREPHTHALIC ACID	200.5	320.0		149.90	16.42	4.86	1
3-CHLOROPHTHALIC ACID	200.5	186.0	9.85	149.90	16.42	4.86	1
4-CHLOROISOPHTHALIC ACID	200.5	295.0		149.90	16.42	4.86	1
4-CHLOROPHTHALIC ACID	200.5	157.0	10.30	149.90	16.42	4.86	1
5-CHLOROISOPHTHALIC ACID	200.5	278.0		149.90	16.42	4.86	2
2-BROMO-4-HYDROXYBENZALDEHYDE	200.9	159.5	9.50	127.50	15.12	5.90	1
2-BROMO-5-HYDROXYBENZALDEHYDE	200.9	135.0	9.35	127.50	15.12	5.90	1
3-BROMO-2-HYDROXYBENZALDEHYDE	200.9	49.0	9.36	127.50	15.12	5.90	1
3-BROMO-4-HYDROXYBENZALDEHYDE	200.9	124.0	9.49	127.50	15.12	5.90	1
4-BROMO-2-HYDROXYBENZALDEHYDE	200.9	52.0	9.91	127.50	15.12	5.90	1
4-BROMO-3-HYDROXYBENZALDEHYDE	200.9	131.5	9.91	127.50	15.12	5.90	1
5-BROMO-2-HYDROXYBENZALDEHYDE	200.9	105.0	9.30	127.50	15.12	5.90	1
M-BROMOBENZOIC ACID	200.9	155.0	10.00	127.10	15.12	3.18	1
O-BROMOBENZOIC ACID	200.9	150.0	9.31	127.10	15.12	3.18	1
P-BROMOBENZOIC ACID	200.9	254.0	10.60	127.10	15.12	3.18	2
2-CHLORO-4-NITROBENZOIC ACID	201.5	140.0	10.49	145.00	16.15	7.20	1
2-CHLORO-5-NITROBENZOIC ACID	201.5	165.0	10.25	145.00	16.15	7.20	1
3-CHLORO-2-NITROBENZOIC ACID	201.5	237.0	9.81	145.00	16.15	7.20	1
3-CHLORO-5-NITROBENZOIC ACID	201.5	147.0	10.30	145.00	16.15	7.20	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
4-CHLORO-2-NITROBENZOIC ACID	201.5	142.0	10.25	145.00	16.15	7.20	1
4-CHLORO-3-NITROBENZOIC ACID	201.5	181.0	10.25	145.00	16.15	7.20	1
M-BROMONITROBENZENE	201.9	56.0	9.18	122.20	14.85	5.52	1
O-BROMONITROBENZENE	201.9	43.0	8.41	122.20	14.85	5.52	1
P-BROMONITROBENZENE	201.9	127.0	9.70	122.20	14.85	5.52	2
FLUORANTHENE	202.0	111.0	11.60	182.60	23.72	0.00	2
PYRENE	202.0	156.0	11.68	182.60	23.72	0.00	4
1,2-DINITRO-4-CHLOROBENZENE	202.5	40.0	9.45	140.10	15.88	9.54	1
1,3-DINITRO-2-CHLOROBENZENE	202.5	88.0	9.45	140.10	15.88	9.54	2
2,3-DINITROCHLOROBENZENE	202.5	78.0	8.95	140.10	15.88	9.54	1
2,4-DINITROCHLOROBENZENE	202.5	53.0	9.45	140.10	15.88	9.54	1
3,5-DINITROCHLOROBENZENE	202.5	59.0	9.45	140.10	15.88	9.54	2
1,2,3,4-TETRAMETHYL-5,6-DICHLOROBENZENE	203.0	193.0	9.18	179.00	20.64	4.76	12
2-PHENANTHRONITRILE	203.0	108.0	13.40	185.50	23.48	3.90	1
3-PHENANTHRONITRILE	203.0	102.0	11.95	185.50	23.48	3.90	1
9-PHENANTHRONITRILE	203.0	103.0	11.59	185.50	23.48	3.90	1
IODOBENZENE	203.9	-31.0	8.74	107.90	14.53	1.30	2
3-CHLORO-2-HYDROXYBIPHENYL	204.5	6.0	11.67	172.80	21.29	3.18	1
4-CHLORO-4'-HYDROXYBIPHENYL	204.5	146.0	13.49	172.80	21.29	3.18	1
5-CHLORO-2-HYDROXYBIPHENYL	204.5	11.0	11.67	172.80	21.29	3.18	1
1,3-DIMETHYLANTHRACENE	206.0	83.0	12.96	201.20	24.82	0.80	1
2,3-DIMETHYLANTHRACENE	206.0	252.0	12.98	201.20	24.82	0.80	2
2,6-DICHLORO-4-ETHOXYANILINE	206.0	46.0	11.38	162.30	19.03	6.34	2
3,4-DICHLOROANTHRANILIC ACID	206.0	237.0	10.24	149.20	17.21	6.33	1
3,5-DICHLORO-4-ETHOXYANILINE	206.0	105.0	11.38	162.30	19.03	6.34	2
3,6-DICHLOROANTHRANILIC ACID	206.0	155.0	9.29	149.20	17.21	6.33	1
4,5-DICHLOROANTHRANILIC ACID	206.0	213.0	10.24	149.20	17.21	6.33	1
4,5-DIMETHYLPHENANTHRENE	206.0	76.0	11.66	201.20	24.82	0.80	2
4-AMINO-3,5-DICHLOROBENZOIC ACID	206.0	291.0	10.02	149.20	17.21	6.33	2
9,10-DIMETHYLANTHRACENE	206.0	181.0	12.05	201.20	24.82	0.80	4

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
9,10-DIMETHYLPHENANTHRENE	206.0	144.0	11.66	201.20	24.82	0.80	2
9-ANTHALDEHYDE	206.0	104.0	11.94	186.20	23.05	2.76	2
9-ETHYLANTHRACENE	206.0	59.0	12.00	200.80	24.82	0.40	2
1-BROMONAPHTHALENE	206.9	-1.0	9.49	142.60	18.48	1.54	1
2-BROMONAPHTHALENE	206.9	59.0	10.79	142.60	18.48	1.54	1
2,6-DICHLORO-4-NITROANILINE	207.0	191.0	9.39	144.30	16.94	8.67	2
1-CHLORO-2-NITRONAPHTHALENE	207.5	81.0	10.63	160.50	19.51	5.56	1
1-CHLORO-3-NITRONAPHTHALENE	207.5	129.5	10.80	160.50	19.51	5.56	1
1-CHLORO-4-NITRONAPHTHALENE	207.5	87.0	9.92	160.50	19.51	5.56	1
1-CHLORO-5-NITRONAPHTHALENE	207.5	111.0	10.19	160.50	19.51	5.56	1
1-CHLORO-6-NITRONAPHTHALENE	207.5	131.0	10.82	160.50	19.51	5.56	1
1-CHLORO-8-NITRONAPHTHALENE	207.5	94.5	9.44	160.50	19.51	5.56	1
2-CHLORO-1-NITRONAPHTHALENE	207.5	99.0	10.58	160.50	19.51	5.56	1
2-CHLORO-3-NITRONAPHTHALENE	207.5	94.5	10.80	160.50	19.51	5.56	1
2-CHLORO-6-NITRONAPHTHALENE	207.5	170.0	11.81	160.50	19.51	5.56	1
2-CHLORO-7-NITRONAPHTHALENE	207.5	136.0	11.51	160.50	19.51	5.56	1
2-CHLORO-8-NITRONAPHTHALENE	207.5	116.0	10.51	160.50	19.51	5.56	1
3-CHLORO-1-NITRONAPHTHALENE	207.5	105.0	10.51	160.50	19.51	5.56	1
3-CHLORO-8-NITRONAPHTHALENE	207.5	100.5	10.69	160.50	19.51	5.56	1
9,10-DIAMINOANTHRACENE	208.0	196.0	11.90	191.00	23.86	3.06	4
2-AMINOISOPHTHALIC ACID DIMETHYL ESTER	209.0	103.0		178.70	19.39	5.99	2
2-AMINOTEREPHTHALIC ACID DIMETHYL ESTER	209.0	134.0		178.70	19.39	5.99	1
4-AMINOPHTHALIC ACID DIMETHYL ESTER	209.0	54.0	10.70	178.70	19.39	5.99	1
2,3,4-TRICHLOROBENZALDEHYDE	209.5	91.0	9.55	143.70	17.19	7.50	1
2,3,5-TRICHLOROBENZALDEHYDE	209.5	56.0	9.30	143.70	17.19	7.50	1
2,3,6-TRICHLOROBENZALDEHYDE	209.5	86.0	9.30	143.70	17.19	7.50	1
2,4,5-TRICHLOROBENZALDEHYDE	209.5	112.0	9.45	143.70	17.19	7.50	1
2,4,6-TRICHLOROBENZALDEHYDE	209.5	58.0	9.55	143.70	17.19	7.50	2
3,4,5-TRICHLOROBENZALDEHYDE	209.5	90.0	9.55	143.70	17.19	7.50	2
1,2,3-TRICARBOXYLIC ACID	210.0	223.0	11.25	162.90	16.92	4.92	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,2,3-TRINITROBENZENE	213.0	82.0	9.45	148.20	16.11	11.94	2
1,2,4-TRINITROBENZENE	213.0	61.0	9.70	148.20	16.11	11.94	1
1,3,5-TRINITROBENZENE	213.0	121.0	9.45	148.20	16.11	11.94	6
2,2'-DIHYDROXY-3,3'-DIMETHYLBIPHENYL	214.0	113.0	11.86	201.20	23.56	4.00	1
2,2'-DIHYDROXY-5,5'-DIMETHYLBIPHENYL	214.0	153.5	11.86	201.20	23.56	4.00	1
2,2'-DIHYDROXY-6,6'-DIMETHYLBIPHENYL	214.0	164.0	11.80	201.20	23.56	4.00	1
2,2'-DIMETHOXYBIPHENYL	214.0	155.0	11.80	197.40	23.66	3.30	1
2-AMINO-4'-NITROBIPHENYL	214.0	159.0	12.90	185.10	22.22	5.51	1
[illegible]-NITROBIPHENYL	214.0	125.0	12.26	185.10	22.22	5.51	1
[illegible]'-DIMETHOXYBIPHENYL	214.0	36.0	13.60	197.40	23.66	3.30	1
3-AMINO-4'-NITROBIPHENYL	214.0	137.0	13.17	185.10	22.22	5.51	1
3-AMINO-4-NITROBIPHENYL	214.0	116.0	12.90	185.10	22.22	5.51	1
3-CARBOXYIC ACID-2-HYDROXYBIPHENYL	214.0	186.0	13.15	185.80	21.79	3.24	1
4,4'-DIHYDROXY-3,3'-DIMETHYLBIPHENYL	214.0	161.0	13.28	201.20	23.56	4.00	1
4,4'-DIMETHOXYBIPHENYL	214.0	173.0	15.90	197.40	23.66	3.30	2
4-AMINO-2'-NITROBIPHENYL	214.0	99.0	12.52	185.10	22.22	5.51	1
4-AMINO-3-NITROBIPHENYL	214.0	170.0	13.17	185.10	22.22	5.51	1
4-AMINO-4'-NITROBIPHENYL	214.0	203.0	13.74	185.10	22.22	5.51	1
5,5'-DIHYDROXY-2,2'-DIMETHYLBIPHENYL	214.0	229.0	11.80	201.20	23.56	4.00	1
2-BROMO-3-NITROTOLUENE	215.9	42.0	9.17	139.60	16.62	5.92	1
2-BROMO-4-NITROTOLUENE	215.9	78.0	9.35	139.60	16.62	5.92	1
2-BROMO-5-NITROTOLUENE	215.9	78.0	9.70	139.60	16.62	5.92	1
2-BROMO-6-NITROTOLUENE	215.9	42.0	9.18	139.60	16.62	5.92	1
3-BROMO-2-NITROTOLUENE	215.9	28.0	8.93	139.60	16.62	5.92	2
3-BROMO-4-NITROTOLUENE	215.9	37.0	9.35	139.60	16.62	5.92	1
3-BROMO-5-NITROTOLUENE	215.9	84.0	9.18	139.60	16.62	5.92	2
4-BROMO-2-NITROTOLUENE	215.9	47.0	9.42	139.60	16.62	5.92	1
4-BROMO-3-NITROTOLUENE	215.9	35.0	9.42	139.60	16.62	5.92	1
5-BROMO-2-NITROTOLUENE	215.9	56.0	9.70	139.60	16.62	5.92	1
1,2,3,4-TETRACHLOROBENZENE	216.0	47.0	9.21	138.40	17.28	6.32	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,2,3,5-TETRACHLOROBENZENE	216.0	54.0	9.21	138.40	17.28	6.32	2
1,2,4,5-TETRACHLOROBENZENE	216.0	140.0	9.21	138.40	17.28	6.32	4
1,2-BENZOFLUORENE	216.0	189.0	13.99	199.60	25.49	0.00	1
2,3-BENZOFLUORENE	216.0	210.0	14.11	199.60	25.49	0.00	1
2,5'-DIHYDROXY-2',5-DIMETHYLBIPHENYL	216.0	158.0	11.80	211.80	24.40	4.00	1
BENZANTHRENE	216.0	84.0	11.86	199.60	25.49	0.00	1
2-BROMO-4-NITROANILINE	216.9	104.5	9.37	134.50	16.14	7.05	1
2-BROMO-5-NITROANILINE	216.9	141.0	9.63	134.50	16.14	7.05	1
3-BROMO-4-NITROANILINE	216.9	175.0	9.36	134.50	16.14	7.05	1
4-BROMO-2-NITROANILINE	216.9	111.5	9.40	134.50	16.14	7.05	1
4-BROMO-3-NITROANILINE	216.9	132.0	9.40	134.50	16.14	7.05	1
5-BROMO-2-NITROANILINE	216.9	151.0	9.67	134.50	16.14	7.05	1
6-BROMO-2-NITROANILINE	216.9	74.5	8.50	134.50	16.14	7.05	1
4-CHLORO-2,6-DINITROANILINE	217.5	147.0	9.18	152.40	17.17	11.07	2
3-IODOTOLUENE	217.9	-27.2	9.35	125.30	16.30	1.70	1
4-IODOTOLUENE	217.9	36.0	9.69	125.30	16.30	1.70	2
1,2-DINITRONAPHTHALENE	218.0	162.0	10.70	168.60	19.74	7.96	1
1,3-DINITRONAPHTHALENE	218.0	147.0	10.70	168.60	19.74	7.96	1
1,5-DINITRONAPHTHALENE	218.0	219.0	10.90	168.60	19.74	7.96	2
1,7-DINITRONAPHTHALENE	218.0	156.0	10.50	168.60	19.74	7.96	1
1,8-DINITRONAPHTHALENE	218.0	173.0	9.06	168.60	19.74	7.96	2
2,2',4,4'-TETRAHYDROXYBIPHENYL	218.0	226.0	13.28	182.60	21.20	6.40	1
2,3-DINITRONAPHTHALENE	218.0	172.0	10.76	168.60	19.74	7.96	2
2,6-DINITRONAPHTHALENE	218.0	278.0	12.13	168.60	19.74	7.96	2
2,7-DINITRONAPHTHALENE	218.0	234.0	12.00	168.60	19.74	7.96	2
3,3',5,5'-TETRAHYDROXYBIPHENYL	218.0	310.0	12.50	182.60	21.20	6.40	2
M-IODOANILINE	218.9	33.0	9.89	120.20	15.82	2.83	1
O-IODOANILINE	218.9	60.0	9.89	120.20	15.82	2.83	1
P-IODOANILINE	218.9	67.0	9.63	120.20	15.82	2.83	2
1,4,7-TRIMETHYLPHENANTHRENE	220.0	72.3	12.99	218.60	26.59	1.20	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,6,7-TRIMETHYLPHENANTHRENE	220.0	123.0	13.00	218.60	26.59	1.20	1
1,2,8-TRIMETHYLPHENANTHRENE	221.0	144.0	12.88	223.90	27.01	1.20	1
1-AMINO-4-BROMONAPHTHALENE	221.9	102.0	9.48	154.90	19.77	3.07	1
1-AMINO-5-BROMONAPHTHALENE	221.9	69.0	10.06	154.90	19.77	3.07	1
2-AMINO-1-BROMONAPHTHALENE	221.9	63.0	10.44	154.90	19.77	3.07	1
2-AMINO-3-BROMONAPHTHALENE	221.9	169.0	10.78	154.90	19.77	3.07	1
2-AMINO-6-BROMONAPHTHALENE	221.9	128.0	11.71	154.90	19.77	3.07	1
3-AMINO-1-BROMONAPHTHALENE	221.9	72.0	10.43	154.90	19.77	3.07	1
6-AMINO-1-BROMONAPHTHALENE	221.9	38.0	10.38	154.90	19.77	3.07	1
P-FLUOROIODOBENZENE	221.9	-27.2	9.52	112.50	14.49	2.76	2
1-BROMO-2-HYDROXYNAPHTHALENE	222.9	84.0	10.51	150.70	19.07	3.14	1
1-BROMO-4-HYDROXYNAPHTHALENE	222.9	128.0	9.49	150.70	19.07	3.14	1
1-BROMO-5-HYDROXYNAPHTHALENE	222.9	137.0	10.09	150.70	19.07	3.14	1
1-BROMO-8-HYDROXYNAPHTHALENE	222.9	61.0	9.49	150.70	19.07	3.14	1
2,2'-DICHLOROBIPHENYL	223.0	61.0	11.55	179.20	22.56	3.16	1
2,4'-DICHLOROBIPHENYL	223.0	43.0	12.51	179.20	22.56	3.16	1
2,4-DICHLOROBIPHENYL	223.0	24.4	12.51	179.20	22.56	3.16	1
2,5-DICHLOROBIPHENYL	223.0	23.0	11.58	179.20	22.56	3.16	1
2-ACETAMIDOFLUORENE	223.0	194.0	14.80	205.80	24.66	3.60	1
2-NITROPHENANTHRENE	223.0	119.0	12.80	189.00	23.37	3.98	1
3,3'-DICHLOROBIPHENYL	223.0	29.0	11.67	179.20	22.56	3.16	1
3-NITROPHENANTHRENE	223.0	172.0	12.23	189.00	23.37	3.98	1
4,4'-DICHLOROBIPHENYL	223.0	148.0	13.77	179.20	22.56	3.16	2
9-NITROANTHRACENE	223.0	146.0	11.93	189.00	23.37	3.98	2
9-NITROPHENANTHRENE	223.0	116.0	11.67	189.00	23.37	3.98	1
1,2,5-TRIMETHYL-3,4,6-TRICHLOROBENZENE	223.5	210.0	9.21	176.10	20.73	5.94	12
1,3,5-TRIMETHYL-2,4,6-TRICHLOROBENZENE	223.5	205.0	9.18	176.10	20.73	5.94	12
1,4-DINITROTETRAMETHYLBENZENE	224.0	211.0	9.70	195.20	21.10	9.56	4
2,3,4-TRICHLOROBENZOIC ACID	225.5	187.0	10.25	151.40	17.78	6.38	1
2,3,5-TRICHLOROBENZOIC ACID	225.5	163.0	9.81	151.40	17.78	6.38	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,3,6-TRICHLOROBENZOIC ACID	225.5	124.0	9.8	151.40	17.78	6.38	1
2,4,5-TRICHLOROBENZOIC ACID	225.5	168.0	10.25	151.40	17.78	6.38	1
2,4,6-TRICHLOROBENZOIC ACID	225.5	164.0	10.25	151.40	17.78	6.38	2
3,4,5-TRICHLOROBENZOIC ACID	225.5	210.0	10.25	151.40	17.78	6.38	2
1,2-DICHLORO-4-BROMOBENZENE	225.9	25.0	9.49	128.60	16.48	4.70	1
1,3-DICHLORO-2-BROMOBENZENE	225.9	65.0	8.41	128.60	16.48	4.70	2
1,4-DICHLORO-2-BROMOBENZENE	225.9	35.0	9.21	128.60	16.48	4.70	1
2,3-DICHLOROBROMOBENZENE	225.9	60.0	8.59	128.60	16.48	4.70	2
3,5-DICHLOROBROMOBENZENE	225.9	83.0	8.59	128.60	16.48	4.70	6
1,2,10-TRIHYDROXYANTHRACENE	226.0	208.0	12.50	190.70	23.05	4.80	1
1,2,9-TRIHYDROXYANTHRACENE	226.0	149.0	12.50	190.70	23.05	4.80	1
1,4,9-TRIHYDROXYANTHRACENE	226.0	156.0	11.95	190.70	23.05	4.80	1
1,8,9-TRIHYDROXYANTHRACENE	226.0	178.0	11.90	190.70	23.05	4.80	2
4,5-DIMETHOXYISOPHTHALIC ACID	226.0	245.0		182.60	19.38	6.58	1
1,2,3-TRICHLORO-5-NITROBENZENE	226.5	72.0	9.45	146.50	17.51	8.72	2
1,3,4-TRICHLORO-2-NITROBENZENE	226.5	89.0	9.21	146.50	17.51	8.72	1
1,3,5-TRICHLORO-2-NITROBENZENE	226.5	71.0	9.45	146.50	17.51	8.72	2
2,3,4-TRICHLORONITROBENZENE	226.5	56.0	9.45	146.50	17.51	8.72	1
2,4,5-TRICHLORONITROBENZENE	226.5	58.0	9.45	146.50	17.51	8.72	1
2,3,4-TRINITROTOLUENE	227.0	112.0	9.70	165.60	17.88	12.34	1
2,3,5-TRINITROTOLUENE	227.0	97.0	9.70	165.60	17.88	12.34	1
2,3,6-TRINITROTOLUENE	227.0	112.0	9.70	165.60	17.88	12.34	1
2,4,5-TRINITROTOLUENE	227.0	104.0	9.70	165.60	17.88	12.34	1
2,4,6-TRINITROTOLUENE	227.0	82.0	9.45	165.60	17.88	12.34	2
3,4,5-TRINITROTOLUENE	227.0	134.0	9.45	165.60	17.88	12.34	2
1,2-BENZANTHRACENE	228.0	162.0	14.00	209.40	27.00	0.00	1
1,2-BENZOPHENANTHRENE	228.0	255.0	13.99	209.40	27.00	0.00	2
1,2-DIMETHOXY-4,5-DINITROBENZENE	228.0	130.0	10.53	172.80	18.84	11.26	2
2,4,6-TRINITROANILINE	228.0	192.0	9.45	160.50	17.40	13.47	2
2,4-DINITRO-3-HYDROXYBENZOIC ACID	228.0	204.0	10.49	161.20	16.97	11.20	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
3,4-BENZOPHENANTHRENE	228.0	68.0	11.87	209.40	27.00	0.00	2
3,5-DINITRO-2-HYDROXYBENZOIC ACID	228.0	182.0	10.26	161.20	16.97	11.20	1
3,5-DINITRO-4-HYDROXYBENZOIC ACID	228.0	248.0	10.17	161.20	16.97	11.20	2
9,10-BENZOPHENANTHRENE	228.0	199.0	11.55	209.40	27.00	0.00	6
NAPHTHACENE	228.0	357.0	14.42	209.40	27.00	0.00	4
2,3,4,5-TETRACHLOROTOLUENE	230.0	98.0	9.21	155.80	19.05	6.72	2
2,3,4,5-TETRACHLOROTOLUENE	230.0	98.1	9.21	155.80	19.05	6.72	2
2,3,4,6-TETRACHLOROTOLUENE	230.0	96.0	9.21	155.80	19.05	6.72	2
2,3,5,6-TETRACHLOROTOLUENE	230.0	93.0	9.21	155.80	19.05	6.72	2
9,10-DIHYDRO-1,2-BENZANTHRACENE	230.0	112.0	14.29	216.60	27.26	0.00	1
9,10-DIHYDRONAPHTHACENE	230.0	212.0	14.42	216.60	27.26	0.00	1
4-AMINO-5-BROMO-2-NITROTOLUENE	230.9	121.0	9.70	151.90	17.91	7.45	1
5-BROMO-4-HYDROXY-3-METHOXYBENZALDEHYDE	230.9	164.0	10.55	151.10	17.53	7.55	1
2,3,4,5-TETRACHLOROANILINE	231.0	118.0	9.29	150.70	18.57	7.85	1
2,3,5,6-TETRACHLOROANILINE	231.0	108.0	9.29	150.70	18.57	7.85	2
1,3-DIMETHYL-2-IODOBENZENE	231.9	11.0	8.96	142.70	18.07	2.10	2
2-IODOBENZALDEHYDE	231.9	37.0	8.74	127.70	16.30	4.06	1
2-IODOBENZALDEHYEDE	231.9	57.0	9.69	127.70	16.30	4.06	1
4-IODOBENZALDEHYDE	231.9	77.0	10.15	127.70	16.30	4.06	2
2-AMINO-4-IODOTOLUENE	232.9	49.0	9.69	137.60	17.59	3.23	1
2-AMINO-5-IODOTOLUENE	232.9	90.0	9.70	137.60	17.59	3.23	1
2-BROMOBIPHENYL	232.9	1.0	11.80	169.40	21.76	1.54	1
3-AMINO-2-IODOTOLUENE	232.9	42.0	8.77	137.60	17.59	3.23	1
3-AMINO-4-IODOTOLUENE	232.9	43.0	9.69	137.60	17.59	3.23	1
3-AMINO-5-IODOTOLUENE	232.9	79.0	9.35	137.60	17.59	3.23	1
4-AMINO-2-IODOTOLUENE	232.9	40.0	9.18	137.60	17.59	3.23	1
4-AMINO-3-IODOTOLUENE	232.9	40.0	9.35	137.60	17.59	3.23	1
4-BROMOBIPHENYL	232.9	91.2	13.00	169.40	21.76	1.54	1
5-AMINO-2-IODOTOLUENE	232.9	46.0	9.70	137.60	17.59	3.23	1
5-BROMOACENAPHTHENE	232.9	52.0	10.12	166.00	21.18	1.54	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1-AMINO-2,4-DINITRONAPHTHALENE	233.0	242.0	10.89	180.90	21.03	9.49	1
2-AMINO-1,6-DINITRONAPHTHALENE	233.0	248.0	11.90	180.90	21.03	9.49	1
1-IODO-4-METHOXYBENZENE	233.9	53.0	11.01	131.50	16.94	2.95	2
2,5-DICHLOROTEREPHTHALIC ACID	235.0	306.0		164.40	18.28	6.44	2
2,7-DICHLOROFLUORENE	235.0	128.0	13.68	185.60	23.49	3.16	1
3,4-DICHLOROPHTHALIC ACID	235.0	195.0		164.40	18.28	6.44	1
4,6-DICHLOROISOPHTHALIC ACID	235.0	280.0		164.40	18.28	6.44	2
2-BROMO-3-CHLOROBENZOIC ACID	235.4	224.0	9.77	141.60	16.98	4.76	1
2-BROMO-5-CHLOROBENZOIC ACID	235.4	153.0	9.74	141.60	16.98	4.76	1
3-BROMO-2-CHLOROBENZOIC ACID	235.4	165.0	10.08	141.60	16.98	4.76	1
3-BROMO-4-CHLOROBENZOIC ACID	235.4	215.0	10.25	141.60	16.98	4.76	1
3-BROMO-6-CHLOROBENZOIC ACID	235.4	155.0	10.04	141.60	16.98	4.76	1
4-BROMO-3-CHLOROBENZOIC ACID	235.4	218.0	10.49	141.60	16.98	4.76	1
M-DIBROMOBENZENE	235.8	-7.0	8.90	118.80	15.68	3.08	2
O-DIBROMOBENZENE	235.8	7.1	8.41	118.80	15.68	3.08	2
P-DIBROMOBENZENE	235.8	87.3	9.73	118.80	15.68	3.08	4
2,2',4,4',6,6'-HEXAMETHYLBIPHENYL	238.0	103.0	13.58	254.60	29.46	2.40	2
M-CHLOROIODOBENZENE	238.4	n.a.	8.90	122.40	16.39	2.88	1
O-CHLOROIODOBENZENE	238.4	n.a.	8.74	122.40	16.39	2.88	1
P-CHLOROIODOBENZENE	238.4	57.0	9.82	122.40	16.39	2.88	2
5-NITROISOPHTHALIC ACID DIMETHYL ESTER	239.0	123.0		189.00	20.19	8.44	2
2-BROMO-4,6-DICHLOROANILINE	240.9	83.5	9.16	140.90	17.77	6.23	1
4-BROMO-2,3-DICHLOROANILINE	240.9	77.5	9.40	140.90	17.77	6.23	1
4-BROMO-2,5-DICHLOROANILINE	240.9	91.0	9.40	140.90	17.77	6.23	1
4-BROMO-3,5-DICHLOROANILINE	240.9	129.0	9.40	140.90	17.77	6.23	2
1,3-DIMETHYL-2,4,6-TRINITROBENZENE	241.0	184.0	9.45	183.00	19.65	12.74	2
1,4-DIMETHYL-2,3,5-TRINITROBENZENE	241.0	140.0	9.45	183.00	19.65	12.74	1
2,4,6-TRINITROBENZALDEHYDE	241.0	119.0	9.86	168.00	17.88	14.70	2
1'-METHYL-1,2-BENZANTHRACENE	242.0	138.0	13.86	226.80	28.77	0.40	1
1-METHYLCHRYSENE	242.0	256.0	14.00	226.80	28.77	0.40	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
10-METHYL-1,2-BENZANTHRACENE	242.0	141.0	14.50	226.80	28.77	0.40	1
2,2'-BIPHENYLDICARBOXYLIC ACID	242.0	233.5	11.80	205.20	23.56	3.28	1
2,2'-DIHYDROXY-3,3',5,5'-TETRAMETHYLBIPH	242.0	113.0	12.70	236.00	27.10	4.80	1
2,2'-DIMETHOXY-5,5'-DIMETHYLBIPHENYL	242.0	71.0	15.90	232.20	27.20	4.10	1
2,3'-BIPHENYLDICARBOXYLIC ACID	242.0	216.0	12.96	205.20	23.56	3.28	1
2,4'-BIPHENYLDICARBOXYLIC ACID	242.0	272.0	13.72	205.20	23.56	3.28	1
2,5'-DIMETHOXY-2',5-DIMETHYLBIPHENYL	242.0	86.0	12.55	232.20	27.20	4.10	1
2-METHYLCHRYSENE	242.0	229.0	14.93	226.80	28.77	0.40	1
3,3'-BIPHENYLDICARBOXYLIC ACID	242.0	356.0	13.45	205.20	23.56	3.28	1
3,4'-BIPHENYLDICARBOXYLIC ACID	242.0	334.0	15.20	205.20	23.56	3.28	1
3,5-BIPHENYLDICARBOXYLIC ACID	242.0	310.0	12.99	205.20	23.56	3.28	1
3-METHYL-1,2-BENZANTHRACENE	242.0	156.0	14.70	226.80	28.77	0.40	1
3-METHYLCHRYSENE	242.0	172.0	14.10	226.80	28.77	0.40	1
4,4'-DIHYDROXY-3,3',5,5'-TETRAMETHYLBIPH	242.0	222.0	13.28	236.00	27.10	4.80	2
4,4'-DIHYDROXY-3,3'-DIETHYLBIPHENYL	242.0	148.0	14.00	235.20	27.10	4.00	1
4,4'-DIMETHOXY-3,3'-DIMETHYLBIPHENY	242.0	145.5	15.98	232.20	27.20	4.10	1
4-METHYL-1,2-BENZANTHRACENE	242.0	126.0	14.05	226.80	28.77	0.40	1
5-METHYL-1,2-BENZANTHRACENE	242.0	160.0	13.86	226.80	28.77	0.40	1
5-METHYLCHRYSENE	242.0	170.0	13.99	226.80	28.77	0.40	1
6-METHYL-1,2-BENZANTHRACENE	242.0	150.0	13.86	226.80	28.77	0.40	1
6-METHYLCHRYSENE	242.0	149.0	13.99	226.80	28.77	0.40	1
7-METHYL-1,2-BENZANTHRACENE	242.0	183.0	13.86	226.80	28.77	0.40	1
8-METHYL-1,2-BENZANTHRACENE	242.0	118.0	13.86	226.80	28.77	0.40	1
9-METHYL-1,2-BENZANTHRACENE	242.0	138.0	14.90	226.80	28.77	0.40	1
2,3,4-TRINITROANISOLE	243.0	155.0	10.61	171.80	18.52	13.59	1
2,3,5-TRINITROANISOLE	243.0	106.8	10.25	171.80	18.52	13.59	1
2,4,5-TRINITROANISOLE	243.0	106.0	10.79	171.80	18.52	13.59	1
2,4,6-TRINITROANISOLE	243.0	69.0	10.60	171.80	18.52	13.59	2
2-HYDROXY-3,4,5-TRINITROTOLUENE	243.0	102.0	9.45	173.70	18.47	13.94	1
3-HYDROXY-2,4,6-TRINITROTOLUENE	243.0	110.0	9.45	173.70	18.47	13.94	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,2'-DINITROBIPHENYL	244.0	127.0	11.67	195.40	23.02	7.96	1
2,3'-DINITROBIPHENYL	244.0	118.0	12.10	195.40	23.02	7.96	1
2,3,4,5-TETRACHLOROBENZALDEHYDE	244.0	106.0	9.55	158.20	19.05	9.08	1
2,4'-DINITROBIPHENYL	244.0	93.0	12.81	195.40	23.02	7.96	1
2,4,5,6-TETRACHLORO-M-XYLENE	244.0	221.0	9.21	173.20	20.82	7.12	12
3,3'-DINITROBIPHENYL	244.0	200.0	12.09	195.40	23.02	7.96	1
4'-HYDROXY-1,2-BENZANTHRACENE	244.0	225.0	14.57	217.50	27.59	1.60	1
4,4'-DIAMINO-3,3'-DIMETHOXYBIPHENYL	244.0	137.0	16.84	222.00	26.24	6.36	1
4,4'-DINITROBIPHENYL	244.0	240.0	14.13	195.40	23.02	7.96	1
5,6-DINITROACENAPHTHENE	244.0	220.0	10.46	192.00	22.44	7.96	1
TETRACHLORO-O-XYLENE	244.0	228.0	9.21	173.20	20.82	7.12	12
2-BROMOFLUORENE	244.9	113.0	12.85	175.80	22.69	1.54	1
2-BROMOTEREPHTHALIC ACID	244.9	299.0		154.60	17.48	4.82	1
4-BROMOISOPHTHALIC ACID	244.9	287.0		154.60	17.48	4.82	1
2-BROMO-3-NITROBENZOIC ACID	245.9	191.0	10.26	149.70	17.21	7.16	1
2-BROMO-4-NITROBENZOIC ACID	245.9	166.0	10.48	149.70	17.21	7.16	1
2-BROMO-5-NITROBENZOIC ACID	245.9	180.0	10.25	149.70	17.21	7.16	1
3-BROMO-2-NITROBENZOIC ACID	245.9	250.0	10.06	149.70	17.21	7.16	1
3-BROMO-4-NITROBENZOIC ACID	245.9	197.0	10.49	149.70	17.21	7.16	1
3-BROMO-5-NITROBENZOIC ACID	245.9	159.0	10.24	149.70	17.21	7.16	1
4-BROMO-2-NITROBENZOIC ACID	245.9	163.0	10.49	149.70	17.21	7.16	1
4-BROMO-3-NITROBENZOIC ACID	245.9	203.0	10.49	149.70	17.21	7.16	1
5-BROMO-2-NITROBENZOIC ACID	245.9	140.0	10.03	149.70	17.21	7.16	1
10-METHYL-1,2-CYCLOHEXANOANTHRACENE	246.0	117.0	13.83	241.20	29.29	0.40	1
2,3,4,5-TETRACHLOROANISOLE	246.0	83.0	10.23	162.00	19.69	7.97	1
2,3,4,6-TETRACHLOROANISOLE	246.0	64.0	10.04	162.00	19.69	7.97	1
2,3,5,6-TETRACHLOROANISOLE	246.0	89.0	9.41	162.00	19.69	7.97	2
2-HYDROXY-3,4,5,6-TETRACHLOROTOLUENE	246.0	190.0	9.21	163.90	19.64	8.32	2
3-HYDROXY-2,4,5,6-TETRACHLOROTOLUENE	246.0	190.0	9.21	163.90	19.64	8.32	2
4-HYDROXY-2,3,5,6-TETRACHLOROTOLUENE	246.0	190.0	9.21	163.90	19.64	8.32	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,2-DINITRO-4-BROMOBENZENE	246.9	60.0	9.70	144.80	16.94	9.50	1
1,3-DINITRO-2-BROMOBENZENE	246.9	107.0	9.45	144.80	16.94	9.50	2
1,4-DINITRO-2-BROMOBENZENE	246.9	70.0	9.70	144.80	16.94	9.50	1
2,3-DINITROBROMOBENZENE	246.9	101.0	9.18	144.80	16.94	9.50	1
2,4-DINTROBROMOBENZENE	246.9	75.0	9.70	144.80	16.94	9.50	1
2-IODOBENZAMID	246.9	183.0	9.2	139.60	17.59	4.92	2
3-IODOBENZAMID	246.9	187.0	10.36	139.60	17.59	4.92	2
4-IODOBENZAMID	246.9	218.0	10.97	139.60	17.59	4.92	4
9,10-DICHLOROANTHRACENE	247.0	212.0	11.93	195.40	25.00	3.16	4
1-CHLORO-2,4,5-TRINITROBENZENE	247.5	116.0	9.18	162.70	17.97	13.52	1
1-CHLORO-2,4,6-TRINITROBENZENE	247.5	83.0	9.53	162.70	17.97	13.52	2
2-IODOBENZOIC ACID	247.9	163.0	9.31	135.40	16.89	2.94	1
3-IODOBENZOIC ACID	247.9	187.0	10.42	135.40	16.89	2.94	1
4-IODOBENZOIC ACID	247.9	228.0	11.05	135.40	16.89	2.94	2
1-IODO-2-NITROBENZENE	248.9	54.0	8.74	130.50	16.62	5.28	1
1-IODO-3-NITROBENZENE	248.9	38.0	9.55	130.50	16.62	5.28	1
1-IODO-4-NITROBENZENE	248.9	174.0	10.10	130.50	16.62	5.28	2
3-BROMO-4-HYDROXYBIPHENYL	248.9	96.0	12.50	177.50	22.35	3.14	1
4-BROMO-4'-HYDROXYBIPHENYL	248.9	164.0	13.76	177.50	22.35	3.14	1
2,5-DIBROMOTOLUENE	249.8	6.0	9.73	136.20	17.45	3.48	1
3,5-DIBROMOTOLUENE	249.8	39.0	8.96	136.20	17.45	3.48	6
PENTACHLOROBENZENE	250.5	86.0	9.21	152.90	19.14	7.90	2
2,3-DIBROMOANILINE	250.8	43.0	8.50	131.10	16.97	4.61	1
2,4-DIBROMOANILINE	250.8	79.5	9.36	131.10	16.97	4.61	1
2,5-DIBROMOANILINE	250.8	53.0	9.80	131.10	16.97	4.61	1
2,6-DIBROMOANILINE	250.8	87.0	8.41	131.10	16.97	4.61	2
3,4-DIBROMOANILINE	250.8	81.0	9.36	131.10	16.97	4.61	1
3,5-DIBROMOANILINE	250.8	57.0	8.41	131.10	16.97	4.61	2
BENZO[A]PYRENE	252.0	177.8	13.90	225.60	29.44	0.00	1
BENZO[E]PYRENE	252.0	176.5	12.00	225.60	29.44	0.00	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
PERYLENE	252.0	277.0	12.05	225.60	29.44	0.00	4
1-IODONAPHTHALENE	253.9	4.2	9.51	150.90	20.25	1.30	1
2-IODONAPHTHALENE	253.9	54.5	11.18	150.90	20.25	1.30	1
1,2,3,4-TETRACARBOXYLIC ACID	254.0	241.0	11.47	190.40	19.28	6.56	2
1,2,4,5-TETRACARBOXYBENZENE	254.0	242.0	11.47	190.40	19.28	6.56	4
3,4'-ACE-1,2-BENZANTHRACENE	254.0	XXXXXX	13.89	232.80	29.70	0.00	1
B-B'-BINAPHTHYL	254.0	187.0	16.48	236.20	30.28	0.00	1
CHOLANTHRENE	254.0	174.5	14.03	232.80	29.70	0.00	1
a,a'-BINAPHTHYL	254.0	144.0	13.90	236.20	30.28	0.00	1
1,2,3-TRINITRO-4,5,6-TRIMETHYLBENZENE	255.0	209.0	9.45	200.40	21.42	13.14	2
1,2,4-TRINITRO-3,5,6-TRIMETHYLBENZENE	255.0	185.0	9.70	200.40	21.42	13.14	1
1,3,5-TRINITRO-2,4,6-TRIMETHYTLBENZENE	255.0	238.0	9.45	200.40	21.42	13.14	6
10-CARBOXALDEHYDE-1,2-BENZANTHRACENE	256.0	148.0	16.30	229.20	28.77	2.76	1
10-ETHYL-1,2-BENZANTHRACENE	256.0	114.0		243.80	30.54	0.40	1
5,6-DIMETHYLCHRYSENE	256.0	128.0	14.00	244.20	30.54	0.80	1
9,10-DIMETHYLBENZANTHRACENE	256.0	122.0	14.90	244.20	30.54	0.80	1
9-BROMOPHENANTHRENE	256.9	64.0	11.66	185.60	24.20	1.54	1
2',3,4-TRICHLOROBIPHENYL	257.5	60.0	12.55	193.70	24.42	4.74	1
2,2',5-TRICHLOROBIPHENYL	257.5	44.0	11.55	193.70	24.42	4.74	1
2,4,4'-TRICHLOROBIPHENYL	257.5	57.0	13.69	193.70	24.42	4.74	1
2,4,5-TRICHLOROBIPHENYL	257.5	77.0	12.51	193.70	24.42	4.74	1
3,4,4'-TRICHLOROBIPHENYL	257.5	88.0	13.69	193.70	24.42	4.74	1
2,3,4,5-TETRACHLOROBENZOIC ACID	260.0	194.0	10.25	165.90	19.64	7.96	1
3-FLUORO-10-METHYL-1,2-BENZANTHRACENE	260.0	n.a.	14.13	231.40	28.73	1.86	1
4-FLUORO-10-METHYL-1,2-BENZANTHRACENE	260.0	n.a.	14.13	231.40	28.73	1.86	1
1-NITRO-2,3,5,6-TETRACHLOROBENZENE	261.0	100.0	9.21	161.00	19.37	10.30	2
2-BROMO-3,5-DINITROANILINE	261.9	181.0	9.63	157.10	18.23	11.03	1
2-BROMO-4,5-DINITROANILINE	261.9	186.0	9.63	157.10	18.23	11.03	1
4-BROMO-2,5-DINITROANILINE	261.9	186.0	9.55	157.10	18.23	11.03	1
4-BROMO-2,6-DINITROANILINE	261.9	163.0	9.40	157.10	18.23	11.03	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
5-BROMO-2,4-DINITROANILINE	261.9	178.4	9.67	157.10	18.23	11.03	1
6-BROMO-2,3-DINITROANILINE	261.9	158.0	9.67	157.10	18.23	11.03	1
1,3,5-TRINITRONAPHTHALENE	263.0	122.0	10.94	191.20	21.83	11.94	1
1,3,8-TRINITRONAPHTHALENE	263.0	218.0	10.93	191.20	21.83	11.94	1
1,4,5-TRINITRONAPHTHALENE	263.0	154.0	10.57	191.20	21.83	11.94	1
1,5-DIBROMO-2,4-DIMETHYLBENZENE	263.8	68.0	9.73	153.60	19.22	3.88	4
1,2-DIMETHOXY-4-IODOBENZENE	263.9	35.0	11.01	155.10	19.35	4.60	1
2-BROMO-4,6-DINITROANILINE	263.9	153.0	9.37	165.70	18.23	11.03	1
PENTACHLOROTOLUENE	264.5	224.0	9.21	170.30	20.91	8.30	12
PENTACHLOROANILINE	265.5	232.0	9.29	165.20	20.43	9.43	2
2,4-DIBROMO-6-HYDROXYTOLUENE	265.8	100.0	9.42	144.30	18.04	5.08	1
3,5-DIBROMO-2-HYDROXYTOLUENE	265.8	58.0	9.20	144.30	18.04	5.08	2
3,6-DIBROMO-2-HYDROXYTOLUENE	265.8	38.0	9.73	144.30	18.04	5.08	1
1,2:5,6-DIBENZOFLUORENE	266.0	174.0	14.53	242.60	31.21	0.00	1
1,2:7,8-DIBENZOFLUORENE	266.0	234.0	15.90	242.60	31.21	0.00	2
5-METHYL-3,4-BENZPYRENE	266.0	216.0	13.89	243.00	31.21	0.40	1
1-AMINO-2-BROMO-4-NITRONAPHTHALENE	266.9	200.0	10.86	177.50	21.86	7.05	1
3,4-BENZOPYRENE-5-AMINO	267.0	239.0	12.00	237.90	30.73	1.53	1
2,2'-DIACETAMIDOBIPHENYL	268.0	164.0	11.67	248.60	28.62	7.20	1
2,4-DIACETAMIDOBIPHENYL	268.0	202.0	14.89	248.60	28.62	7.20	1
20-METHYLCHOLANTHRENE	268.0	177.0	14.02	250.20	31.47	0.40	1
3,4-BENZOPYRENE-5-HYDROXY	268.0	207.0	12.00	233.70	30.03	1.60	1
3,4-BENZOPYRENE-8-HYDROXY(DEC)	268.0	226.0	13.00	233.70	30.03	1.60	1
4,4'-DIACETAMIDOBIPHENYL	268.0	328.3	18.66	248.60	28.62	7.20	2
2-AMINO-3-IODONAPHTHALENE	268.9	137.0	11.14	163.20	21.54	2.83	1
2,2'-BIPHENYLDICARBOXYL DIMETHYLESTER	270.0	74.0	11.80	236.20	27.10	4.46	1
2,2'-DIETHOXY-3,3'-DIMETHYLBIPHENYL	270.0	85.0	11.74	266.20	30.74	4.10	1
2,4'-DIETHOXY-3,3'-DIMETHYLBIPHENYL	270.0	53.0	15.14	266.20	30.74	4.10	1
3,3'-BIPHENYLDICARBOXYLIC DIMETHYL ESTER	270.0	104.0	15.90	236.20	27.10	4.46	1
3,4'-BIPHENYLDICARBOXYLIC DIMETHYL ESTER	270.0	98.0	16.90	236.20	27.10	4.46	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
3,5-BIPHENYLDICARBOXYLIC DIMETHYL ESTER	270.0	214.0	14.24	236.20	27.10	4.46	1
4,4'-DIETHOXY-3,3'-DIMETHYLBIPHENYL	270.0	156.0	17.80	266.20	30.74	4.10	1
4-NITROPHTHALIC ACID DIMETHYL ESTER	271.0	69.0		201.40	21.47	10.94	1
1,3-DICHLORO-5-IODOBENZENE	272.9	57.0	8.90	136.90	18.25	4.46	2
1,4-DICHLORO-2-IODOBENZENE	272.9	21.0	9.21	136.90	18.25	4.46	1
3,3'-DIETHYL-6,6'-DIHYDROXY	274.0	131.0	13.63	247.60	28.38	6.50	1
BENZ(G,H,I)PERYLENE	276.0	279.0	12.05	241.80	31.88	0.00	2
6-CHLORO-10-METHYL-1,2-BENZANTHRACENE	276.5	n.a.	15.12	241.30	30.63	1.98	1
2,3-DIBROMO-1,4,5-TRIMETHYLBENZENE	277.8	63.0	9.42	171.00	20.99	4.28	2
2,4-DIBROMO-1,3,5-TRIMETHYLBENZENE	277.8	66.0	9.42	171.00	20.99	4.28	2
4-HYDROXY-2-IODO-3-METHOXYBENZALDEHYDE	277.9	155.0	10.36	159.40	19.30	7.31	1
4-HYDROXY-5-IODO-3-METHOXYBENZALDEHYDE	277.9	180.0	10.45	159.40	19.30	7.31	1
1,2:3,4-DIBENZANTHRACENE	278.0	205.0	14.00	252.40	32.72	0.00	2
1,2:5,6-DIBENZANTHRACENE	278.0	269.0	16.20	252.40	32.72	0.00	2
1,2:6,7-DIBENZANTHRACENE	278.0	263.0	16.20	252.40	32.72	0.00	1
1,2:6,7-DIBENZOPHENANTHRENE	278.0	294.0	16.30	252.40	32.72	0.00	1
1,2:7,8-DIBENZANTHRACENE	278.0	197.0	14.50	252.40	32.72	0.00	2
2,3:6,7-DIBENZOPHENANTHRENE	278.0	257.0	16.20	252.40	32.72	0.00	2
PENTACENE	278.0	270.0	16.95	252.40	32.72	0.00	4
PICENE	278.0	364.0	16.50	252.40	32.72	0.00	2
PENTACHLOROBENZALDEHYDE	278.5	202.5	9.55	172.70	20.91	10.66	2
2,3-DIBROMOBENZOIC ACID	279.8	149.0	10.07	146.30	18.04	4.72	1
2,4-DIBROMOBENZOIC ACID	279.8	174.0	10.57	146.30	18.04	4.72	1
2,5-DIBROMOBENZOIC ACID	279.8	157.0	10.07	146.30	18.04	4.72	1
2,6-DIBROMOBENZOIC ACID	279.8	150.0	9.12	146.30	18.04	4.72	2
3,4-DIBROMOBENZOIC ACID	279.8	234.0	10.49	146.30	18.04	4.72	1
3,5-DIBROMO-2-HYDROXYBENZALDEHYDE	279.8	82.0	9.38	146.70	18.04	7.44	1
4-IODOBIPHENYL	279.9	113.0	13.35	177.70	23.53	1.30	1
5-IODOACENAPHTHENE	279.9	65.0	10.50	174.30	22.95	1.30	1
1,2-DIBROMO-3-NITROBENZENE	280.8	85.0	9.18	141.40	17.77	7.06	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,2-DIBROMO-4-NITROBENZENE	280.8	59.0	9.70	141.40	17.77	7.06	1
1,3-DIBROMO-2-NITROBENZENE	280.8	84.0	8.90	141.40	17.77	7.06	2
1,3-DIBROMO-5-NITROBENZENE	280.8	106.0	9.18	141.40	17.77	7.06	2
1,4-DIBROMO-2-NITROBENZENE	280.8	86.0	9.73	141.40	17.77	7.06	1
2,4-DIBROMO-1-NITROBENZENE	280.8	62.0	9.70	141.40	17.77	7.06	1
3,5-DIBROMO-4-METHOXYANILINE	280.8	66.0	9.79	154.70	19.38	6.26	2
M-BROMOIODOBENZENE	282.8	-9.3	9.25	127.10	17.45	2.84	1
O-BROMOIODOBENZENE	282.8	10.0	8.74	127.10	17.45	2.84	1
P-BROMOIODOBENZENE	282.8	92.0	10.03	127.10	17.45	2.84	2
10-BUTYL-1,2-BENZANTHRACENE	284.0	97.0		277.80	34.08	0.40	1
HEXACHLOROBENZENE	285.0	230.0	9.21	167.40	21.00	9.48	12
2,2'-DIHYDROXY-a,a'-BINAPHTHYL	286.0	220.0	13.90	252.40	31.46	3.20	1
4,4'-DIHYDROXY-a,a'-BINAPHTHYL	286.0	200.0	13.90	252.40	31.46	3.20	1
4,4'-DIAMINO-3,3'-DIMETHYLa,a'BINAPHTHYL	288.0	213.0	13.90	279.40	33.96	3.86	1
2,2',3,3'-TETRACHLOROBIPHENYL	292.0	121.0	12.20	208.20	26.28	6.32	1
2,2',3,5'-TETRACHLOROBIPHENYL	292.0	47.0	12.55	208.20	26.28	6.32	1
2,2',4,4'-TETRACHLOROBIPHENYL	292.0	42.0	13.69	208.20	26.28	6.32	1
2,2',5,5'-TETRACHLOROBIPHENYL	292.0	87.0	12.15	208.20	26.28	6.32	1
2,3',4',5-TETRACHLOROBIPHENYL	292.0	106.0	13.69	208.20	26.28	6.32	1
2,3',4,4'-TETRACHLOROBIPHENYL	292.0	128.0	13.69	208.20	26.28	6.32	1
2,3,4,5-TETRACHLOROBIPHENYL	292.0	92.0	12.60	208.20	26.28	6.32	1
3,3',4,4'-TETRACHLOROBIPHENYL	292.0	183.0	13.69	208.20	26.28	6.32	1
2-IODO-4-NITROBENZOIC ACID	292.9	146.0	10.49	158.00	18.98	6.92	1
4-IODO-2-NITROBENZOIC ACID	292.9	192.0	10.90	158.00	18.98	6.92	1
4-IODO-3-NITROBENZOIC ACID	292.9	213.0	10.90	158.00	18.98	6.92	1
5-IODO-3-NITROBENZOIC ACID	292.9	167.0	10.37	158.00	18.98	6.92	2
PENTACHLOROBENZOIC ACID	294.5	208.0	10.25	180.40	21.50	9.54	2
4,6-DIBROMO-2-ETHOXYANILINE	294.8	52.0	10.00	171.70	21.15	6.26	1
PENTACHLORO-NITROBENZENE	295.5	144.0	9.45	175.50	21.23	11.88	2
2,4-DIBROMO-6-NITROANILINE	295.8	128.0	9.36	153.70	19.06	8.59	1

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
10-PENTYL-1,2-BENZANTHRACENE	298.0	83.0		294.80	35.85	0.40	1
4-4'-DIETHOXY-3,3'-DIETHYLBIPHENYL	298.0	120.0	17.80	300.20	34.28	4.10	1
PENTACARBOXYBENZENE	298.0	238.0	11.47	217.90	21.64	8.20	2
CORONENE	300.0	439.0	12.01	258.00	34.32	0.00	12
1-AMINO-2,4-DIBROMONAPHTHALENE	300.8	118.0	10.81	174.10	22.69	4.61	1
2-AMINO-1,4-DIBROMONAPHTHALENE	300.8	106.0	10.41	174.10	22.69	4.61	1
2-AMINO-1,6-DIBROMONAPHTHALENE	300.8	121.0	11.67	174.10	22.69	4.61	1
1,2:4,5-DIBENZOPYRENE	302.0	233.0	13.98	268.60	35.16	0.00	1
15,16-BENZDEHYDROCHOLANTHRENE	302.0	181.0	15.15	268.60	35.16	0.00	1
4,4'-DIHYDROXY-3,3',5,5'-TETRAMETHOXYBIP	306.0	222.0	14.60	260.80	29.66	9.80	2
1,3,5,8-TETRANITRONAPHTHALENE	308.0	194.0	10.65	213.80	23.92	15.92	1
1,3,6,8-TETRANITRONAPHTHALENE	308.0	207.0	11.34	213.80	23.92	15.92	2
1,2:5,6-DIBENZANTHRACENE-4',4''-DIHYDROX	310.0	415.0	16.60	268.60	33.90	3.20	2
4,4'-DIBROMOBIPHENYL	311.8	164.0	14.30	188.60	24.68	3.08	2
4,4'-DICHLORO-2,2'-DINITROBIPHENYL	313.0	140.0	13.77	224.40	26.74	11.12	1
1,2,3-TRIBROMOBENZENE	314.7	87.0	8.90	138.00	18.60	4.62	2
1,2,4-TRIBROMOBENZENE	314.7	44.0	9.73	138.00	18.60	4.62	1
1,3,5-TRIBROMOBENZENE	314.7	122.0	8.90	138.00	18.60	4.62	6
2,2'-DICARBOXY-3,3'-DIMETHYL-4-NITROBIPH	315.0	217.0	13.30	262.60	29.19	8.06	1
2,2'-DICARBOXY-3,3'-DIMETHYL-5-NITROBIPH	315.0	267.0	13.00	262.60	29.19	8.06	1
2,2',3,4,5'-PENTACHLOROBIPHENYL	326.5	112.0	12.55	222.70	28.14	7.90	1
2,2',3,4,5-PENTACHLOROBIPHENYL	326.5	100.0	12.51	222.70	28.14	7.90	1
2,2',3,4,6-PENTACHLOROBIPHENYL	326.5	100.0	12.51	222.70	28.14	7.90	1
2,2',4,5,5'-PENTACHLOROBIPHENYL	326.5	77.0	12.55	222.70	28.14	7.90	1
2,3,4,5,6-PENTACHLOROBIPHENYL	326.5	124.0	12.51	222.70	28.14	7.90	1
HEXACENE	328.0	380.0	19.50	295.40	38.44	0.00	4
2,3,4-TRIBROMOTOLUENE	328.7	46.0	9.42	155.40	20.37	5.02	2
2,3,5-TRIBROMOTOLUENE	328.7	54.0	9.73	155.40	20.37	5.02	2
2,3,6-TRIBROMOTOLUENE	328.7	61.0	9.73	155.40	20.37	5.02	2
2,4,5-TRIBROMOTOLUENE(114)	328.7	82.0	9.73	155.40	20.37	5.02	4

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,4,6-TRIBROMOTOLUENE	328.7	70.0	9.42	155.40	20.37	5.02	2
2,4,5-TRIBROMOANILINE	329.7	80.0	9.80	150.30	19.89	6.15	1
2,4,6-TRIBROMOANILINE	329.7	122.0	9.27	150.30	19.89	6.15	2
3,4,5-TRIBROMOANILINE	329.7	123.0	9.27	150.30	19.89	6.15	2
M-DIIODOBENZENE	329.8	40.0	9.55	135.40	19.22	2.60	2
O-DIIODOBENZENE	329.8	27.0	8.74	135.40	19.22	2.60	2
P-DIIODOBENZENE	329.8	132.0	10.50	135.40	19.22	2.60	4
2,2',4,4'-TETRANITROBIPHENYL	334.0	165.0	13.96	240.60	27.20	15.92	1
9,10-DIBROMOANTHRACENE	335.8	226.0	11.94	204.80	27.12	3.08	4
HEXACARBOXYBENZENE(DEC)	342.0	286.0	11.47	245.40	24.00	9.84	12
1,3,5-TRIBROMOANISOLE	344.7	88.0	10.65	161.60	21.01	6.27	2
2,3,4-TRIBROMOANISOLE	344.7	106.0	10.58	161.60	21.01	6.27	1
2,3,5-TRIBROMOANISOLE	344.7	82.0	9.83	161.60	21.01	6.27	1
2,4,5-TRIBROMOANISOLE	344.7	105.0	10.67	161.60	21.01	6.27	1
3,4,5-TRIBROMOANISOLE	344.7	91.0	10.67	161.60	21.01	6.27	2
2,4-DIIODOANILINE	344.8	95.0	9.75	147.70	20.51	4.13	1
2,5-DIIODOANILINE	344.8	88.0	10.52	147.70	20.51	4.13	1
2,6-DIIODOANILINE	344.8	122.0	8.85	147.70	20.51	4.13	2
3,4-DIIODOANILINE	344.8	74.5	9.75	147.70	20.51	4.13	1
3,5-DIIODOANILINE	344.8	110.0	9.83	147.70	20.51	4.13	2
9,9'-BIFLUORENYL	346.0	247.0		373.00	43.10	0.00	2
2,4,6-TRIBROMO-1,3,5-TRIMETHYLBENZENE	356.7	227.0	9.42	190.20	23.91	5.82	12
2,3,4-TRIBROMOBENZOIC ACID	358.7	197.0	10.49	165.50	20.96	6.26	1
2,3,5-TRIBROMOBENZOIC ACID	358.7	193.0	10.08	165.50	20.96	6.26	1
2,4,5-TRIBROMOBENZOIC ACID	358.7	195.0	10.49	165.50	20.96	6.26	1
2,4,6-TRIBROMOBENZOIC ACID	358.7	198.0	10.49	165.50	20.96	6.26	2
3,4,5-TRIBROMOBENZOIC ACID	358.7	240.0	10.49	165.50	20.96	6.26	2
1,2,3-TRIBROMO-5-NITROBENZENE	359.7	112.0	9.70	160.60	20.69	8.60	2
1,3,4-TRIBROMO-2-NITROBENZENE	359.7	185.0	9.73	160.60	20.69	8.60	1
1,3,5-TRIBROMO-2-NITROBENZENE	359.7	125.0	9.70	160.60	20.69	8.60	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
2,3,4-TRIBROMONITROBENZENE	359.7	85.0	9.70	160.60	20.69	8.60	1
2,3,5-TRIBROMO-NITROBENZENE	359.7	120.0	9.73	160.60	20.69	8.60	1
2,4,5-TRIBROMONITROBENZENE	359.7	95.0	9.73	160.60	20.69	8.60	1
2,2',3,3',4,4'-HEXACHLOROBIPHENYL	361.0	157.0	13.69	237.20	30.00	9.48	1
2,2',3,3',4,5-HEXACHLOROBIPHENYL	361.0	85.0	12.55	237.20	30.00	9.48	1
2,2',3,3',5,6-HEXACHLOROBIPHENYL	361.0	100.0	12.18	237.20	30.00	9.48	1
2,2',4,4',5,5'-HEXACHLOROBIPHENYL	361.0	103.0	13.69	237.20	30.00	9.48	1
2,2',4,4',6,6'-HEXACHLOROBIPHENYL	361.0	114.0	13.69	237.20	30.00	9.48	2
4,4'-DIHYDROXY-3,3',5,5'-TETRANITROBIPHE	366.0	223.0	13.26	256.80	28.38	19.12	1
3-AMINO-2,4,6-TRIBROMOBENZOIC ACID	373.7	171.5	10.62	177.80	22.25	7.79	1
3,5-DIIODO-4-HYDROXYBENZALDEHYDE	373.8	206.5	9.67	163.30	21.58	6.96	2
2-AMINO-1,3,6-TRIBROMONAPHTHALENE	379.7	143.0	11.62	193.30	25.61	6.15	1
9,10-DIPHENYLNAPHTHACENE	380.0	207.0	16.00	349.00	45.00	0.00	1
9,11-DIPHENYLNAPHTHACENE	380.0	301.0	16.35	349.00	45.00	0.00	1
3,5-DIIODOANTHRANILIC ACID	388.8	232.0	9.60	175.20	22.87	5.77	2
2,4-DIIODO-5-NITROANILINE	389.8	125.0	9.75	170.30	22.60	8.11	1
2,6-DIIODO-3-NITROANILINE	389.8	122.0	10.00	170.30	22.60	8.11	1
2,6-DIIODO-4-NITROANILINE	389.8	245.0	9.33	170.30	22.60	8.11	2
4,6-DIIODO-2-NITROANILINE	389.8	154.0	9.75	170.30	22.60	8.11	1
4,6-DIIODO-3-NITROANILINE	389.8	149.0	10.04	170.30	22.60	8.11	1
1,2,3,5-TETRABROMOBENZENE	393.6	100.0	9.73	157.20	21.52	6.16	2
1,2,4,5-TETRABROMOBENZENE	393.6	182.0	9.73	157.20	21.52	6.16	4
2,2',3,4,5,5',6-HEPTACHLOROBIPHENYL	395.5	149.0	12.05	251.70	31.86	11.06	1
OCTACHLORONAPHTHALENE	404.0	197.0	11.60	239.40	30.44	12.64	4
2,3,5,6-TETRABROMOTOLUENE	407.6	117.0	9.73	174.60	23.29	6.56	2
1,2-DIMETHYL-TETRABROMOBENZENE	421.6	262.0	9.73	192.00	25.06	6.96	12
1,3-DIMETHYL-TETRABROMOBENZENE	421.6	250.0	9.73	192.00	25.06	6.96	12
2,3,4,6-TETRABROMOANISOLE	423.6	113.0	10.57	180.80	23.93	7.81	1
2-HYDROXY-3,4,5,6-TETRABROMOTOLUENE	423.6	208.0	9.73	182.70	23.88	8.16	2
3-HYDROXY-2,4,5,6-TETRABROMOTOLUENE	423.6	194.0	9.73	182.70	23.88	8.16	2

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
4-HYDROXY-2,3,5,6-TETRABROMOTOLUENE	423.6	209.0	9.73	182.70	23.88	8.16	2
2,2',3,3',4,4'5,5'-OCTACHLOROBIPHENYL	430.0	159.0	13.69	266.20	33.72	12.64	1
2,2',3,3',5,5',6,6'-OCTACHLOROBIPHENYL	430.0	162.0	12.10	266.20	33.72	12.64	2
1,2,3-TRIIODOBENZENE	455.7	116.0	9.55	162.90	23.91	3.90	2
1,2,4-TRIIODOBENZENE	455.7	91.0	10.50	162.90	23.91	3.90	1
1,3,5-TRIIODOBENZENE	455.7	184.0	9.55	162.90	23.91	3.90	6
9,10,11-TRIPHENYLNAPHTHACENE	456.0	236.0	16.35	418.80	54.00	0.00	1
2,2',3,3',4,4',5,5',6-NONACHLOROBIPHENYL	464.5	206.0	13.69	280.70	35.58	14.22	1
2,3,4-TRIIODOTOLUENE	469.7	92.0	9.69	180.30	25.68	4.30	1
2,3,5-TRIIODOTOLUENE	469.7	73.0	10.50	180.30	25.68	4.30	1
2,3,6-TRIIODOTOLUENE	469.7	80.0	10.50	180.30	25.68	4.30	1
2,4,5-TRIIODOTOLUENE	469.7	119.0	10.50	180.30	25.68	4.30	1
2,4,6-TRIIODOTOLUENE	469.7	118.0	9.69	180.30	25.68	4.30	2
3,4,5-TRIIODOTOLUENE	469.7	119.0	9.69	180.30	25.68	4.30	2
2,3,5-TRIIODOANILINE	470.7	116.0	10.50	175.20	25.20	5.43	1
2,3,6-TRIIODOANILINE	470.7	116.8	10.50	175.20	25.20	5.43	1
2,4,6-TRIIODOANILINE	470.7	185.5	9.63	175.20	25.20	5.43	2
PENTABROMOBENZENE	472.5	160.0	9.73	176.40	24.44	7.70	2
TETRABROMOISOPHTHALIC ACID	481.6	288.0		212.20	26.24	9.44	2
TETRABROMOTEREPHTHALIC ACID	481.6	266.0		212.20	26.24	9.44	4
2,4,6-TRIIODOANISOLE	485.7	98.0	11.02	186.50	26.32	5.55	2
PENTABROMOTOLUENE	486.5	288.0	9.73	193.80	26.21	8.10	12
PENTABROMOANILINE	487.5	265.0	9.80	188.70	25.73	9.23	2
DECACHLOROBIPHENYL	499.0	305.0	13.69	295.20	37.44	15.80	2
2,3,5-TRIIODOBENZOIC ACID	499.7	224.0	10.37	190.40	26.27	5.54	2
1,3,4-TRIIODO-2-NITROBENZENE	500.7	137.0	10.50	185.50	26.00	7.88	1
2,3,5-TRIIODONITROBENZENE	500.7	124.0	10.50	185.50	26.00	7.88	1
2,4,5-TRIIODONITROBENZENE	500.7	178.0	10.50	185.50	26.00	7.88	1
5-NITRO-1,2,3-TRIIODOBENZENE	500.7	167.0	10.10	185.50	26.00	7.88	2
HEXABROMOBENZENE	551.4	327.0	9.73	195.60	27.36	9.24	12

COMPOUND NAME	MW	MP	LENGTH	VOLUME	ALPHA	SUMDM	SIGMA
1,2,3,4-TETRAIODOBENZENE	581.6	136.0	10.50	190.40	28.60	5.20	2
1,2,3,5-TETRAIODOBENZENE	581.6	148.0	10.50	190.40	28.60	5.20	2
1,2,4,5-TETRAIODOBENZENE	581.6	254.0	10.55	190.40	28.60	5.20	4
PENTAIODOBENZENE	707.5	172.0	10.50	217.90	33.29	6.50	2
HEXAIODOBENZENE	833.4	350.0	10.50	245.40	37.98	7.80	12

APPENDIX C

EXPERIMENTAL DATA FOR FLEXIBLE ORGANIC COMPOUNDS

COMPOUND	$\triangle H_f$ (experimental) (cal/mole)	$\triangle S_f$ (experimental)	TM (°K)	log ϕ	log σ	$\triangle H_f$ (predicted) (cal/mole)	$\triangle S_f$ (predicted)	TM (°K)
n-PROPANE	842.1	9.9	85	0.000	0.301	298.6	7.4	79
2-METHYLPROPANE	1086.1	9.6	113	0.000	0.477	110.0	7.3	90
n-BUTANE	1607.7	12.9	107	0.477	0.301	1099.5	9.8	111
n-PENTANE	2007.2	14.0	143	0.954	0.301	1900.5	12.2	137
2-METHYLBUTANE	1229.7	10.9	113	0.477	0.000	910.9	9.9	103
n-HEXANE	3129.2	17.6	175	1.431	0.301	2701.4	14.6	159
2-METHYLPENTANE	1500.0	12.5	119	0.954	0.000	1712.0	12.3	127
2,3-DIMETHYLBUTANE	1741.6	12.7	136	0.477	0.301	722.3	9.8	119
2,2-DIMETHYLBUTANE	1433.0	11.0	127	0.000	0.000	866.4	7.5	130
n-HEPTANE	3354.1	18.4	182	1.908	0.301	3502.4	17.0	178
2,2,3-TRIMETHYLBUTANE	1126.8	7.0	121	0.000	0.000	677.8	7.5	134
2,4-DIMETHYLPENTANE	1641.1	10.6	154	0.954	0.301	1523.2	12.2	144
2,2-DIMETHYLPENTANE	1390.0	9.3	149	0.477	0.000	1667.2	9.9	154
3,3-DIMETHYLPENTANE	1689.0	12.2	139	0.954	0.301	1667.3	12.2	157
2-METHYLHEXANE	2201.0	14.2	155	1.431	0.000	2512.7	14.8	148
3-ETHYLPENTANE	2279.9	14.8	154	1.431	0.477	2512.7	14.5	171
n-OCTANE	4959.3	22.9	216	2.386	0.301	4303.2	19.4	194
2-METHYLHEPTANE	2839.7	17.3	164	1.908	0.000	3313.6	17.2	166
3,3-DIMETHYLHEXANE	1701.0	11.6	147	1.431	0.000	2468.2	14.8	162
4-METHYLHEPTANE	2590.9	17.0	152	1.908	0.000	3313.6	17.2	166
2,2-DIMETHYLHEXANE	1619.6	10.7	152	0.954	0.000	2468.2	12.3	174
2,5-DIMETHYLHEXANE	3100.5	17.0	182	1.431	0.301	2324.2	14.6	165

3-METHYLHEPTANE	2779.9	18.2	153	1.908	0.000	3313.6	17.2	166
2,2,3-TRIMETHYLPENTANE	2059.8	12.8	161	0.477	0.000	1478.7	9.9	158
2,2,4-TRIMETHYLPENTANE	2198.6	13.3	166	0.477	0.000	1478.7	9.9	158
2,3,3-TRIMETHYLPENTANE	2059.8	13.2	164	0.954	0.000	1478.7	12.3	146
2,3,4-TRIMETHYLPENTANE	2220.1	13.5	164	0.954	0.000	1334.6	12.3	134
2,2,3,3-TETRAMETHYLBUTANE	2275.1	8.0	152	0.000	0.778	633.2	7.1	211
2-METHYL-3-ETHYLPENTANE	2710.5	17.1	158	1.431	0.000	2324.2	14.8	151
3-METHYL-3-ETHYLPENTANE	2588.5	14.2	182	1.431	0.477	2468.2	14.5	188
4-METHYLOCTANE	3827.8	23.9	160	2.386	0.000	4114.6	19.6	182
n-NONANE	5215.3	23.8	216	2.863	0.301	5104.2	21.9	208
3-METHYLOCTANE	4067.0	24.2	165	2.386	0.000	4114.6	19.6	182
3-ETHYL-2,4-DIMETHYLPENTANE	1722.5	11.4	151	1.431	0.000	2135.6	14.8	154
2,2,4-TRIMETHYLHEXANE	2799.0	18.3	153	0.954	0.000	2279.6	12.3	178
2,2,3,3-TETRAMETHYLPENTANE	980.9	4.6	174	0.477	0.000	1434.0	9.9	174
2,2-DIMETHYLHEPTANE	2129.2	13.4	160	1.431	0.000	3269.1	14.8	192
3-ETHYLHEPTANE	3827.8	23.7	158	2.386	0.000	4114.6	19.6	182
2,2,3,4-TETRAMETHYLPENTANE	119.6	0.8	152	0.477	0.000	1290.0	9.9	161
4,4-DIMETHYLHEPTANE	2416.3	.	.	1.908	0.301	3269.1	17.0	195
3,3,4-TRIMETHYLHEXANE	1937.8	11.3	172	1.431	0.000	2279.7	14.8	166
3,5-DIMETHYLHEPTANE	2679.4	.	.	1.908	0.301	3125.1	17.0	184
2,2,3,4-TETRAMETHYLPENTANE	2320.6	11.2	206	0.000	0.301	1434.1	7.4	212
3,3-DIETHYLPENTANE	2464.1	10.4	208	1.908	0.602	3269.1	16.9	214
3-ETHYL-4-METHYLHEXANE	2942.6	.	.	1.908	0.000	3125.1	17.2	169
3-ETHYL-3-METHYLHEXANE	2631.6	.	.	1.908	0.000	3269.1	17.2	180
2,3,4-TRIMETHYLHEXANE	2559.8	.	.	1.431	0.000	2135.5	14.8	154
4-ETHYL-2-METHYLHEXANE	2679.4	.	.	1.908	0.000	3125.1	17.2	169
2,4,4-TRIMETHYLHEXANE	2703.3	17.0	159	1.431	0.000	2279.6	14.8	166

2,2,5-TRIMETHYLHEXANE	1483.3	8.9	167	0.954	0.000	2279.6	13.2	178
3-ETHYL-2-METHYLHEXANE	3110.0	.	.	1.908	0.000	3125.1	17.2	169
2,6-DIMETHYLHEPTANE	3110.0	18.9	170	1.908	0.301	3125.1	17.0	184
2,2,3-TRIMETHYLHEXANE	2464.1	.	.	0.954	0.000	2279.6	12.3	178
3,4-DIMETHYLHEPTANE	3110.0	.	.	1.908	0.000	3125.1	17.2	169
2,3,3,4-TETRAMETHYLPENTANE	2153.1	12.5	171	0.954	0.301	1290.0	12.2	165
3-ETHYL-2,3-DIMETHYLPENTANE	2631.6	.	.	1.431	0.000	2279.6	14.8	166
2,3-DIMETHYLHEPTANE	3349.3	22.2	156	1.908	0.000	3125.1	17.2	169
3,3-DIMETHYLHEPTANE	2846.9	.	.	1.908	0.000	3269.1	17.2	180
3-ETHYL-2,2-DIMETHYLPENTANE	2440.2	14.1	174	0.954	0.000	2279.6	12.3	178
2-METHYLOCTANE	4306.2	22.2	193	2.386	0.000	4114.6	19.6	182
n-DECANE	6866.0	28.2	243	3.340	0.301	5905.1	24.3	221
2,2,5,5-TETRAMETHYLHEXANE	2344.5	9.0	260	0.477	0.301	2235.0	9.8	232
3-ISOPROPYL-2,4-DIMETHYLPENTANE	143.5	0.7	191	0.954	0.477	1946.9	12.1	198
2,7-DIMETHYLOCTANE	4138.8	20.8	219	2.386	0.301	3926.0	19.4	200
2,2,3,4,4-PENTAMETHYLPENTANE	861.2	3.7	234	0.000	0.000	1245.5	7.5	194
3,4,5-TRIMETHYLHEPTANE	3349.3	.	.	1.908	0.000	2936.5	17.2	172
2,3,4-TRIMETHYLHEPTANE	3349.3	.	.	1.908	0.000	2936.5	17.2	172
5-METHYLNONANE	3971.3	21.3	186	2.863	0.000	4915.6	22.0	196
3-ISOPROPYL-3-METHYLHEXANE	2631.6	.	.	1.908	0.000	3080.4	17.2	183
3-METHYLNONANE	4497.6	23.9	188	2.863	0.000	4915.6	22.0	196
2,3,6-TRIMETHYLHEPTANE	3349.3	.	.	1.908	0.000	2936.4	17.2	172
2,2,3,3,4-PENTAMETHYLPENTANE	645.9	2.7	237	0.477	0.000	1245.5	9.9	178
3,3-DIETHYLHEXANE	3588.5	.	.	1.908	0.000	4070.1	17.2	207
4-ETHYLOCTANE	4545.5	.	.	2.862	0.000	4915.6	22.0	196
2,4,5-TRIMETHYLHEPTANE	3110.0	.	.	1.908	0.000	2936.5	17.2	172
2,3-DIMETHYLOCTANE	4306.2	.	.	2.385	0.000	2279.6	19.6	185

3,4-DIETHYLHEXANE	3588.5	.	.	2.385	0.301	3926.1	19.4	200
3-ETHYL-3-METHYLHEPTANE	3588.5	.	.	2.385	0.000	4070.1	19.6	195
2,5,5-TRIMETHYLHEPTANE	2631.6	.	.	1.431	0.000	3080.4	14.8	195
3-ETHYL-4-METHYLHEPTANE	3827.8	.	.	2.385	0.000	3926.1	19.6	185
3-ETHYL-2,2-DIMETHYLHEXANE	3349.3	.	.	1.431	0.000	3080.5	14.8	195
3-ETHYL-5-METHYLHEPTANE	3349.3	.	.	2.385	0.000	3926.1	19.6	185
3,3,5-TRIMETHYLHEPTANE	3349.3	.	.	1.908	0.000	3080.5	17.2	183
4-ETHYL-2-METHYLHEPTANE	3588.5	.	.	2.385	0.000	3926.1	19.6	185
3-ETHYL-2,3-DIMETHYLHEXANE	3349.3	.	.	1.908	0.000	3080.5	17.2	183
4-ETHYL-3-METHYLHEPTANE	3827.8	.	.	2.385	0.000	3926.1	19.6	185
2,3,5-TRIMETHYLHEPTANE	3110.0	.	.	1.908	0.000	2936.5	17.2	172
4-ETHYL-4-METHYLHEPTANE	3349.3	.	.	2.385	0.000	4070.1	19.6	195
2,4,6-TRIMETHYLHEPTANE	2631.6	.	.	1.908	0.000	2936.4	17.2	172
3,6-DIMETHYLOCTANE	3588.5	.	.	2.385	0.301	3926.1	19.4	200
3,3,4-TRIMETHYLHEPTANE	3110.0	.	.	1.908	0.000	3080.5	17.2	183
2,4-DIMETHYLOCTANE	3827.8	.	.	2.385	0.000	3926.1	19.6	185
2,3,3-TRIMETHYLHEPTANE	3588.5	.	.	1.908	0.000	3080.5	17.2	183
5-ETHYL-2-METHYLHEPTANE	3588.5	.	.	2.385	0.000	3926.1	19.6	185
2,4,4-TRIMETHYLHEPTANE	3349.3	.	.	1.908	0.000	3080.5	17.2	183
2,2,4-TRIMETHYLHEPTANE	3588.5	.	.	1.431	0.000	3080.5	14.8	195
3-ETHYL-2,4-DIMETHYLHEXANE	2392.3	.	.	1.908	0.000	2936.5	17.2	172
3-ETHYL-2,5-DIMETHYLHEXANE	3110.0	.	.	1.908	0.000	2936.5	17.2	172
2-METHYLNONANE	4186.6	21.1	198	2.863	0.000	4915.6	22.0	196
3-ETHYL-3,4-DIMETHYLHEXANE	3110.0	.	.	1.908	0.000	3080.5	17.2	183
3-ETHYL-2,2,3-TRIMETHYLPENTANE	1411.5	6.1	231	0.954	0.000	2234.9	12.3	193
4-ETHYL-2,2-DIMETHYLHEXANE	3588.5	.	.	1.431	0.000	3080.5	14.8	195
2,2-DIMETHYLOCTANE	4067.0	.	.	1.908	0.000	4070.0	17.2	207

4-ETHYL-2,3-DIMETHYLHEXANE	3349.3	.	.	1.908	0.000	2936.5	17.2	172
2,5-DIMETHYLOCTANE	3827.8	.	.	2.385	0.000	3926.0	19.6	185
2,3,4,5-TETRAMETHYLHEXANE	2870.8	.	.	1.431	0.301	1946.9	14.6	172
3,5-DIMETHYLOCTANE	3588.5	.	.	2.385	0.000	3926.1	19.6	185
3,3,4,4-TETRAMETHYLHEXANE	2392.3	.	.	1.431	0.301	2235.0	14.6	197
4-ISOPROPYLHEPTANE	3827.8	.	.	2.385	0.000	3926.0	19.6	185
4-ETHYL-3,3-DIMETHYLHEXANE	3110.0	.	.	1.908	0.000	3080.5	17.2	183
4-N-PROPYLHEPTANE	4306.2	.	.	2.862	0.477	4443.1	21.8	202
3,3-DIETHYL-2-METHYLPENTANE	1435.4	.	.	1.431	0.000	3080.4	14.8	195
2,2,3-TRIMETHYLHEPTANE	3349.3	.	.	1.431	0.000	3080.5	14.8	195
2,2,3,4-TETRAMETHYLHEXANE	2153.1	.	.	0.954	0.000	2091.0	12.3	181
3,4,4-TRIMETHYLHEPTANE	2870.8	.	.	1.908	0.000	3080.4	17.2	183
3-ETHYL-2,2,4-TRIMETHYLPENTANE	1435.4	.	.	0.954	0.000	2090.9	12.3	181
3-ETHYLOCTANE	4784.7	.	.	2.862	0.000	4915.6	22.0	196
2,2,4,4-TETRAMETHYLHEXANE	3110.0	.	.	0.954	0.000	2235.0	12.3	193
3,3-DIMETHYLOCTANE	3827.8	.	.	2.385	0.000	4070.1	19.6	195
3-ETHYL-2,3,4-TRIMETHYLPENTANE	478.5	.	.	1.431	0.000	2090.9	14.8	169
2,6-DIMETHYLOCTANE	3827.8	.	.	2.385	0.000	3926.0	19.6	185
2,3,3,4-TETRAMETHYLHEXANE	2870.8	.	.	1.431	0.000	2091.0	14.8	169
2,2,5-TRIMETHYLHEPTANE	2870.8	.	.	1.431	0.000	3080.4	14.8	195
3-ETHYL-2-METHYLHEPTANE	4067.0	.	.	2.385	0.000	3926.0	19.6	185
4,5-DIMETHYLOCTANE	3827.8	.	.	2.385	0.000	3926.0	19.6	185
3,4-DIMETHYLOCTANE	4067.0	.	.	2.385	0.000	3926.0	19.6	185
4-METHYLNONANE	3636.4	20.9	174	2.863	0.000	4915.6	22.0	196
2,3,4,4-TETRAMETHYLHEXANE	2153.1	.	.	1.431	0.000	2091.0	14.8	169
4-ETHYL-2,4-DIMETHYLHEXANE	3588.5	.	.	1.908	0.000	3080.5	17.2	183
2,2,3,3-TETRAMETHYLHEXANE	2966.5	13.5	219	0.954	0.000	2235.0	12.3	193

2,2,3,5-TETRAMETHYLHEXANE	2392.3	.	.	0.954	0.000	2091.0	12.3	181
2,2,4,5-TETRAMETHYLHEXANE	3349.3	.	.	0.954	0.000	2091.0	12.3	181
2,3,3,5-TETRAMETHYLHEXANE	3588.5	.	.	1.431	0.000	2091.0	14.8	169
n-UNDECANE	6937.8	28.3	236	3.817	0.301	6706.0	26.7	233
4-METHYLDECANE	.	.	181	3.339	0.000	5716.5	24.4	209
3-ETHYL-2,2,3-TRIMETHYLHEXANE	.	.	163	1.431	0.000	3035.9	14.8	209
2,2,4,6,6-PENTAMETHYLHEPTANE	1100.5	5.3	202	0.954	0.000	2046.4	12.3	197
n-DODECANE	8588.5	32.6	263	4.294	0.301	7506.9	29.1	243
2-METHYLUNDECANE	.	.	226	3.816	0.000	6517.5	26.8	220
2,5-DIMETHYLDECANE	.	.	189	3.339	0.000	5527.8	24.4	211
5-ETHYL-2-METHYLNONANE	.	.	157	3.339	0.000	5527.8	24.4	211
2,2,7,7-TETRAMETHYLOCTANE	.	.	319	1.431	0.301	3836.8	14.6	261
3,3,6,6-TETRAMETHYLOCTANE	.	.	200	2.385	0.301	3836.8	19.4	227
4-ETHYL-4-N-PROPYLHEPTANE	.	.	203	2.862	0.000	5671.8	22.0	233
4-ISOPROPYL-2,6-DIMETHYLHEPTANE	.	.	171	2.385	0.000	3548.8	19.6	191
2,2,4,4,6-PENTAMETHYLHEPTANE	.	.	190	1.431	0.000	2847.4	14.8	213
2,3,4,5,6-PENTAMETHYLHEPTANE	.	.	193	1.908	0.000	2559.3	17.2	178
n-TRIDECANE	6811.0	25.4	268	4.770	0.301	8307.9	31.5	252
n-TETRADECANE	10772.7	38.6	279	5.247	0.301	9108.8	33.9	260
n-PENTADECANE	8267.9	29.2	283	5.724	0.301	9909.6	36.3	268
n-HEXADECANE	12753.6	43.8	291	6.201	0.301	10710.6	38.8	275
n-HEPTADECANE	9598.1	32.5	295	6.678	0.301	11511.5	41.2	281
n-OCTADECANE	14779.9	49.1	301	7.155	0.301	12312.4	43.6	287
n-NONADECANE	10949.8	35.9	305	7.632	0.301	13113.4	46.0	292
n-EICOSANE	16701.0	53.9	310	8.109	0.301	13914.3	48.4	297
n-21-ALKANE	.	.	313	8.586	0.301	14715.1	50.8	302
n-26-ALKANE	.	.	329	10.971	0.301	18719.9	62.9	321

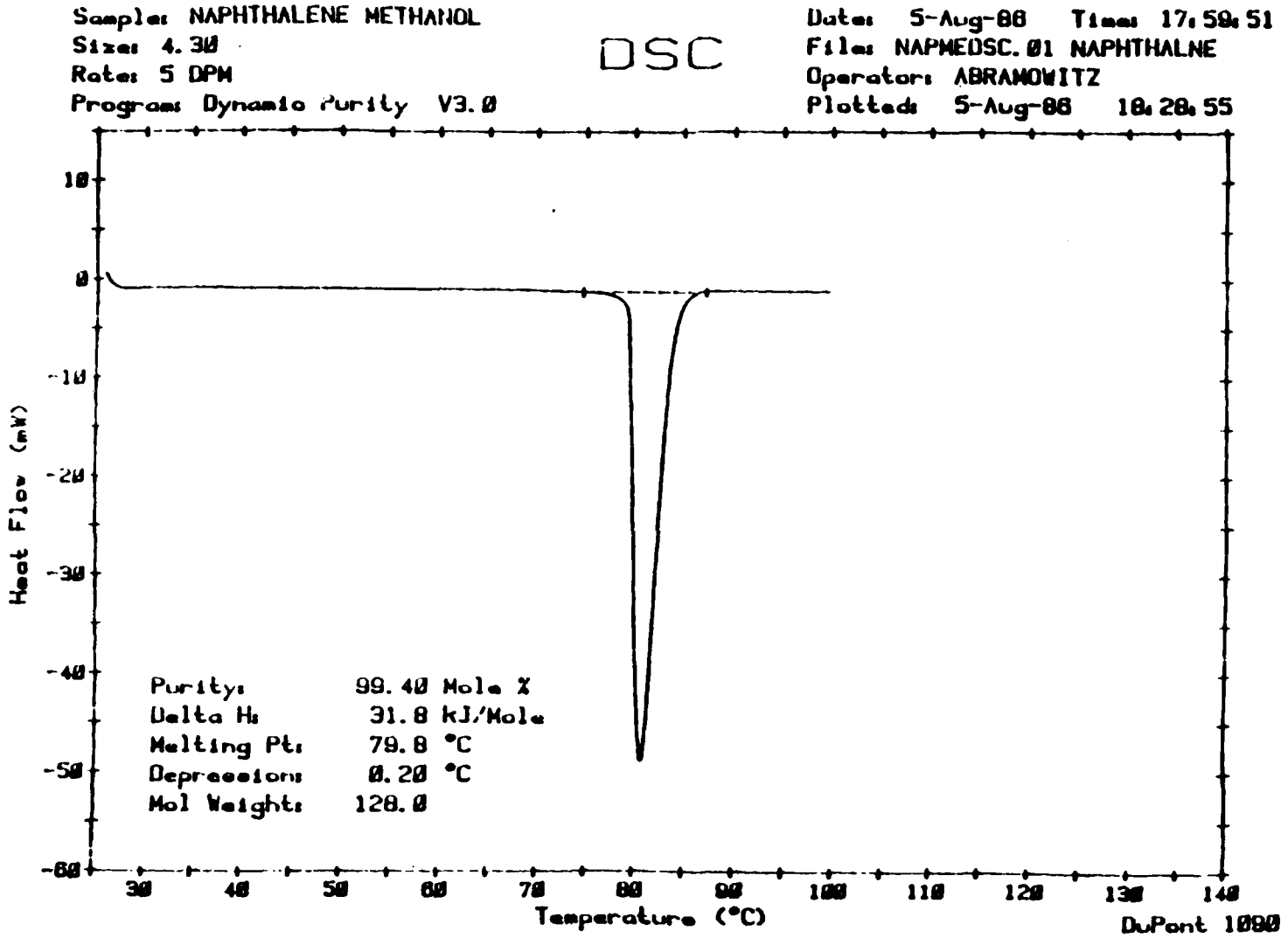
n-27-ALKANE	. .	333	11.448	0.301	19520.8	65.3	324
n-28-ALKANE	. .	337	11.925	0.301	20321.5	67.7	327
n-31-ALKANE	. .	341	12.879	0.301	22724.4	72.6	344
n-44-ALKANE	. .	360	19.557	0.301	33136.4	106.4	359
n-46-ALKANE	. .	361	20.511	0.301	34738.3	111.2	362
n-50-ALKANE	. .	365	22.419	0.301	37941.9	120.9	366
n-52-ALKANE	. .	367	23.373	0.301	39543.8	125.7	368
n-54-ALKANE	. .	368	24.327	0.301	41145.5	130.5	370
n-60-ALKANE	. .	372	27.189	0.301	45951.0	145.0	376
n-62-ALKANE	. .	374	28.143	0.301	47552.9	149.9	377
n-64-ALKANE	. .	375	29.097	0.301	49154.8	154.7	379
n-56-ALKANE	. .	377	30.051	0.301	50756.5	159.5	380
n-67-ALKANE	. .	377	30.528	0.301	51557.4	161.9	381
n-70-ALKANE	. .	379	31.959	0.301	53960.3	169.2	382
n-82-ALKANE	. .	384	37.683	0.301	63571.3	198.2	389
n-94-ALKANE	. .	387	43.407	0.301	73182.3	227.1	393
n-100-ALKANE	. .	388	46.269	0.301	77987.8	241.6	395

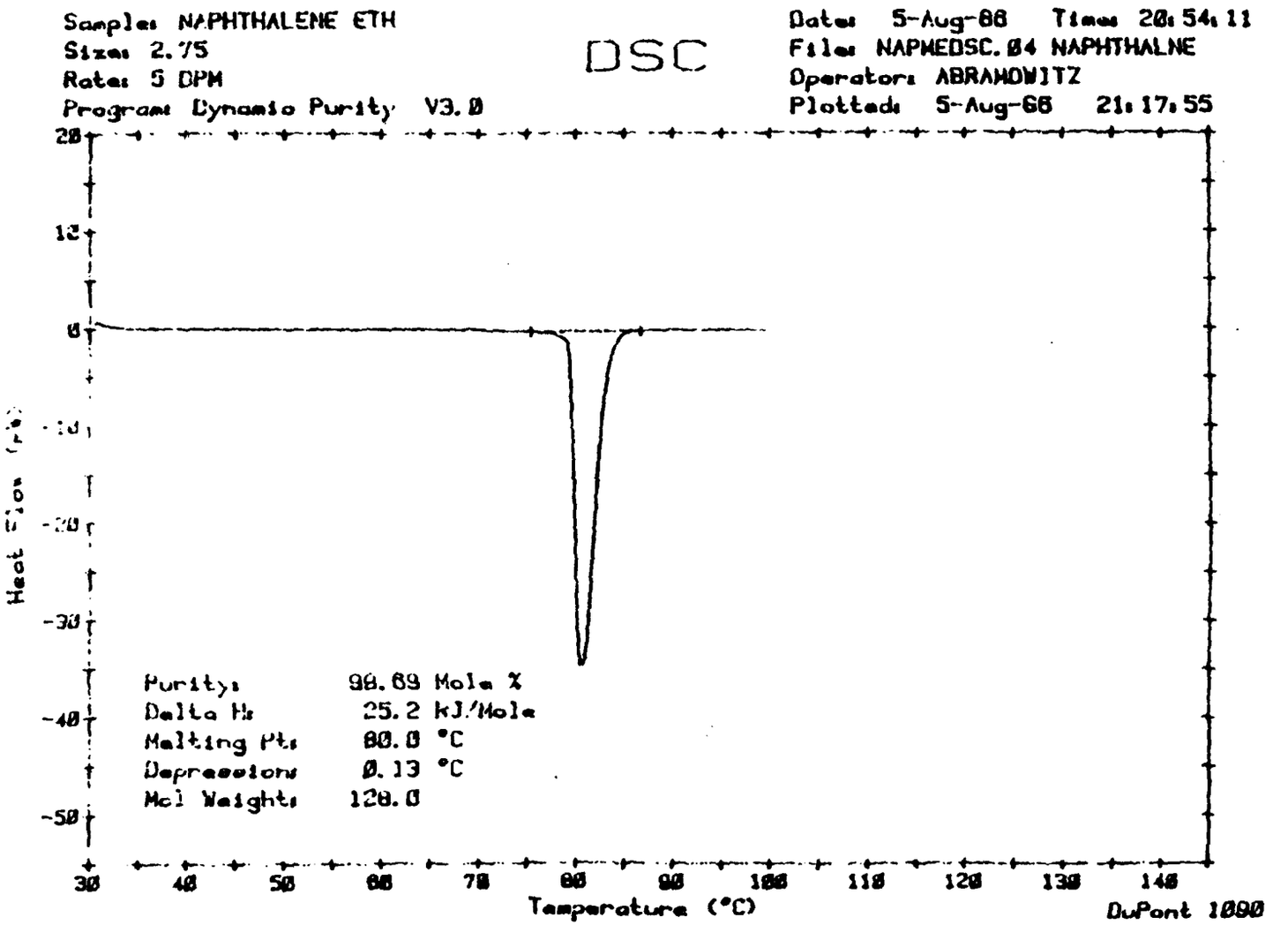
APPENDIX D

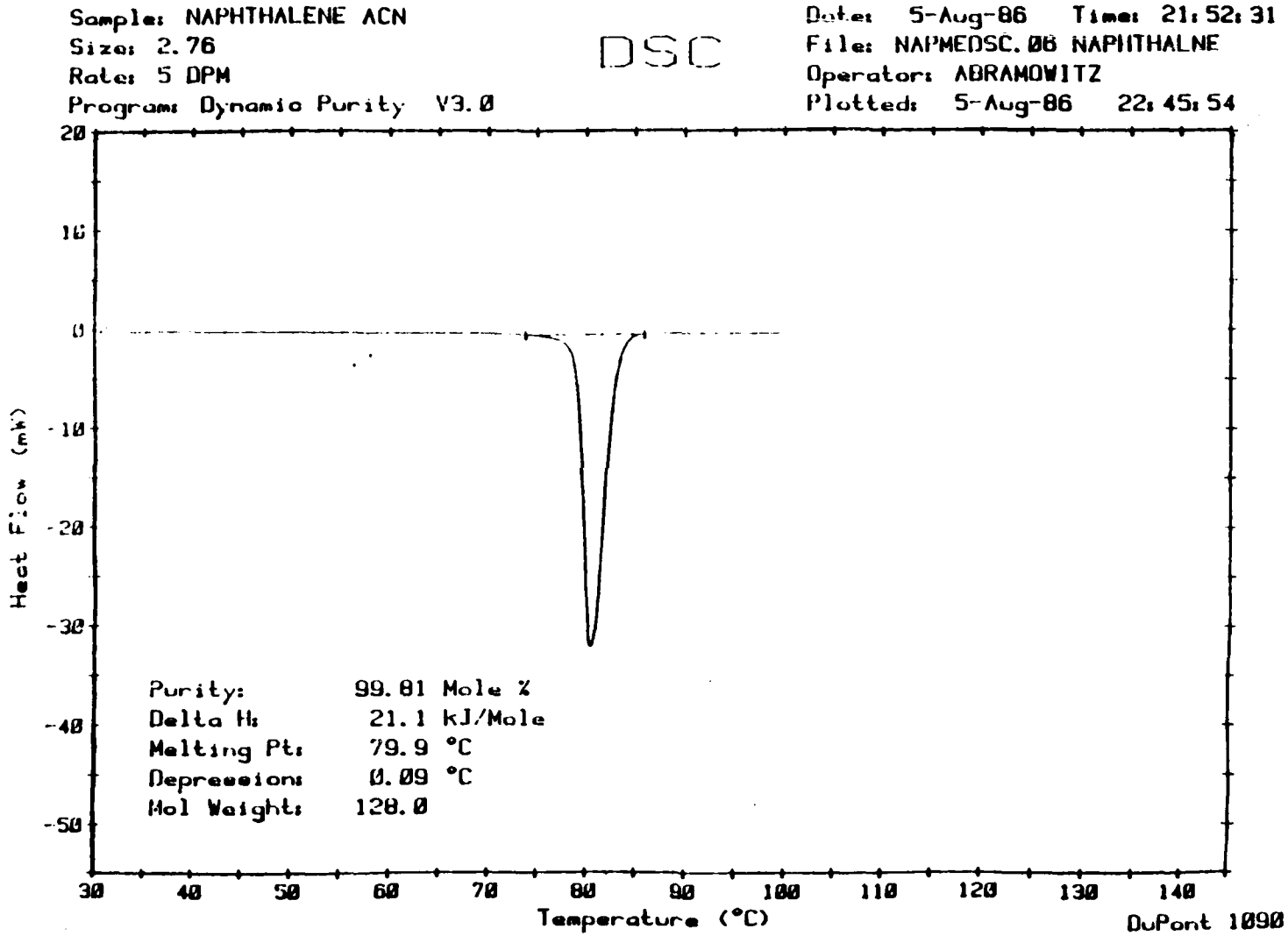
DSC ANALYSES OF ORGANIC COMPOUNDS

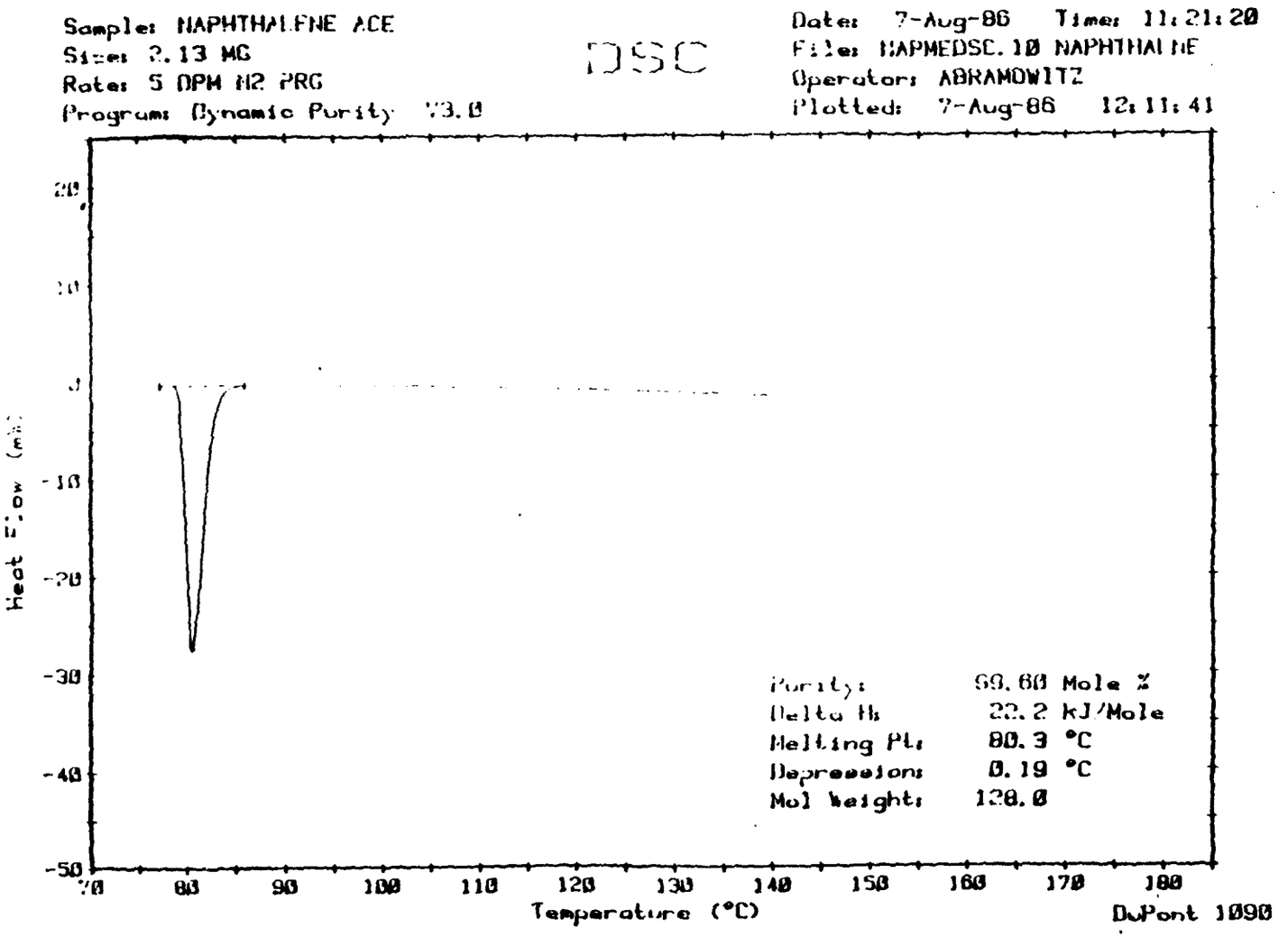
DSC EXPERIMENTAL DATA

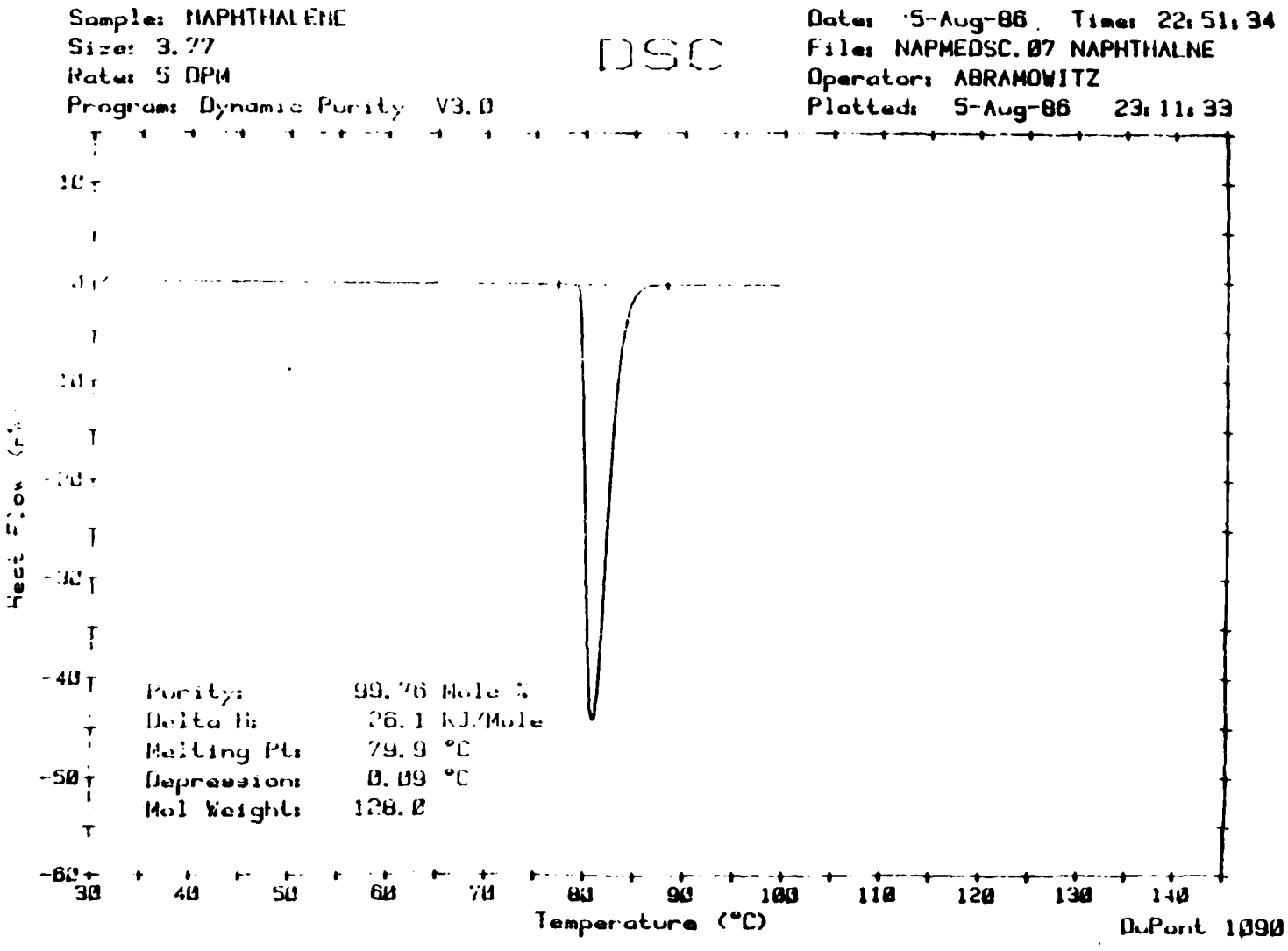
COMPOUND NAME	ENTHALPY OF FUSION (KJ/Mole)	MP (Exp) (°C)	MP (Calc Eq. 15) (°C)
3-AMINOPHENOL	21.6	121.8	78.1
p-BROMOANILINE	15.3	62.3	75.5
p-BROMOBENZOIC ACID	37.7	254.5	179.7
o-BROMOBENZOIC ACID	22.9	149.0	134.1
BENZO(a)PYRENE	15.0	178.6	163.2
1-CHLORO-4-IODOBENZENE	16.5	52.9	50.9
BENZOIC ACID	18.6	122.3	130.7
4-CHLOROPHENOL	5.9	43.3	78.4
p-DIBROMOBENZENE	44.8	87.1	85.6
3,5-DINITROBENZOIC ACID	11.7	207.4	236.3
2,5-DIHYDROXYBENZOIC ACID	65.0	204.3	176.7
HEXAMETHYLBENZENE	17.4	166.0	154.5
4-HYDROXYBENZOIC ACID	20.1	215.0	215.7
2-IODOANILINE	15.5	55.6	59.5
4-IODOANILINE	15.6	62.4	88.2
o-IODOBENZOIC ACID	22.1	161.5	151.7
1-IODO-2-NITROBENZENE	16.4	49.0	43.7
1-IODO-4-NITROBENZENE	14.6	172.7	88.1
o-IODOPHENOL	17.7	40.3	69.8
m-IODOPHENOL	15.2	39.5	71.8
4-IODOPHENOL	16.7	92.2	101.3
2,7-NAPTHALENEDIOL	21.9	188.9	132.8
m-NITROBENZOIC ACID	20.3	142.1	167.6
PHENOL	10.9	40.5	40.7
PICENE		364.0	292.0
PERYLENE	25.5	277.1	193.7
RESORCINOL	10.4	109.5	95.8
SALICYLIC ACID	17.0	159.2	177.6
1,2,4,5-TETRABROMOBENZENE	27.9	182.1	150.9
1,3,5-TRIBROMOBENZENE	62.2	121.7	124.7
1,2,4-TRIBROMOBENZENE		39.0	40.4


Sample: NAPHTHALENE METHANOL
Size: 4.30
Rate: 5 DPM
Program: Dynamic Purity V3.0
DSC
Date: 5-Aug-88 Time: 17:59:51
File: NAPMEDSC.01 NAPHTHALNE
Operator: ABRAMOWITZ
Plotted: 5-Aug-88 18:28:55
Purity: 99.40 Mole %
Delta H: 31.8 kJ/Mole
Melting Pt: 79.8 °C
Depression: 0.20 °C
Mol Weight: 128.0
Heat Flow (mW)
10
0
-10
-20
-30
-40
-50
-60
30
40
50
60
70
80
90
100
110
120
130
140
Temperature (°C)
DuPont 1090


Sample: NAPHTHALENE ETH
Size: 2.75
Rate: 5 DPM
Program: Dynamic Purity V3.0
DSC
Date: 5-Aug-88 Time: 20:54:11
File: NAPMEDSC.04 NAPHTHALNE
Operator: ABRAMOWITZ
Plotted: 5-Aug-88 21:17:55
Heat Flow (mW)
20
10
0
-10
-20
-30
-40
-50
30
40
50
60
70
80
90
100
110
120
130
140
Temperature (°C)
Purity: 98.69 Mole %
Delta H: 25.2 kJ/Mole
Melting Pt: 80.0 °C
Depression: 0.13 °C
Mol Weight: 128.0
DuPont 1090


Sample: NAPHTHALENE ACN
Size: 2.76
Rate: 5 DPM
Program: Dynamic Purity V3.0
DSC
Date: 5-Aug-86 Time: 21:52:31
File: NAPMEDSC.08 NAPHTHALNE
Operator: ABRAMOWITZ
Plotted: 5-Aug-86 22:45:54
Heat Flow (mW)
20
10
0
-10
-20
-30
-40
-50
30
40
50
60
70
80
90
100
110
120
130
140
Temperature (°C)
Purity: 99.81 Mole %
Delta H: 21.1 kJ/Mole
Melting Pt: 79.9 °C
Depression: 0.09 °C
Mol Weight: 128.0
DuPont 1090


Sample: NAPHTHALENE ACE
Size: 2.13 MG
Rate: 5 DPM N2 PRG
Program: Dynamic Purity V3.0
DSC
Date: 7-Aug-86 Time: 11:21:20
File: NAPMEDSC.10 NAPHTHALENE
Operator: ABRAMOWITZ
Plotted: 7-Aug-86 12:11:41
Heat Flow (mW)
20
10
0
-10
-20
-30
-40
-50
70
80
90
100
110
120
130
140
150
160
170
180
Temperature (°C)
Purity: 99.80 Mole %
Delta H: 22.2 kJ/Mole
Melting Pt: 80.3 °C
Depression: 0.19 °C
Mol Weight: 128.0
DuPont 1090


Sample: NAPHTHALENE
Size: 3.77
Rate: 5 DPM
Program: Dynamic Purity V3.0
DSC
Date: 5-Aug-86 Time: 22:51:34
File: NAPMEDSC.07 NAPHTHALNE
Operator: ABRAMOWITZ
Plotted: 5-Aug-86 23:11:33
Purity: 99.76 Mole %
Delta H: 26.1 KJ/Mole
Melting Pt: 79.9 °C
Depression: 0.09 °C
Mol Weight: 128.2
-40
-50
-60
30
40
50
60
70
80
90
100
110
120
130
140
Temperature (°C)
DuPont 1090

APPENDIX E

RIGID COMPOUNDS-SAMPLE CALCULATIONS

EXAMPLE I

COMPOUND: BENZENE
TMPN-(TABLE 6) = 0
TIHBN-(TABLE 7) = 0
TPACK-(TABLE 8) = 0
SIGMA-(APPENDIX B) = 12
SIGMAL = 1.08
LENGTH-(APPENDIX B) = 7.07
VOLUME-(APPENDIX B) = 80.40
EXPAN-(EQUATION 4) = 2.3
$TM_{(experimental)}$-(APPENDIX B) = 5.5 + 273 = 278.5 ^{o}K

Using Equation 15

$TM_{(predicted)}$ = 8.89*2.3 + 73.1*1.08 + 196.3
$TM_{(predicted)}$ = 295.7 ^{o}K

EXAMPLE II

COMPOUND: P-XYLENE
TMPN-(TABLE 6) = 15.08
TIMBN-(TABLE 7) = 0
TPACK-(TABLE 8) = 9.5
SIGMA-(APPENDIX B) = 4
SIGMAL = 0.602
LENGTH-(APPENDIX B) = 9.08
VOLUME-(APPENDIX B) = 115.20
EXPAN-(EQUATION 4) = 3.4
$TM_{(experimental)}$-(APPENDIX B) = 286.0 ^{o}K

Using Equation 15

$TM_{(predicted)}$ = 15.08 + 9.5 + 8.89*3.4 + 73.1*0.602 + 196.3
$TM_{(predicted)}$ = 295.1 ^{o}K

APPENDIX F

FLEXIBLE COMPOUNDS-SAMPLE CALCULATIONS

EXAMPLE I

COMPOUND: n-HEPTANE
log(ϕ)-(APPENDIX C) = 1.908
log(σ)=SIGMAL-(APPENDIX C) = 0.301
$TM_{(experimental)}$-(APPENDIX C) = 182.0 ^{o}K

Using Equation 26

$$TM_{(predicted)} = \frac{1188.7*5 + 944.6*2 - 817.4}{31.9 + 5.8*\ 1.908 - 11.4*0.301}$$

$$TM_{(predicted)} = 178.0\ ^{o}K$$

EXAMPLE II

COMPOUND: 2-METHYLHEPTANE
log(ϕ)-(APPENDIX C) = 1.908
log(σ)=SIGMAL-(APPENDIX C) = 0
$TM_{(experimental)}$-(APPENDIX C) = 164.0 ^{o}K

Using Equation 26

$$TM_{(predicted)} = \frac{370.8*1 + 1188.7*4 + 944.6*3 - 817.4}{31.9 + 5.8*1.908}$$

$$TM_{(predicted)} = 166.0\ ^{o}K$$

END

9-87

DTIC